

COARSENING IN STOCHASTICALLY PERTURBED GINZBURG-LANDAU-TYPE  
EQUATIONS AND STATISTICAL STUDIES OF THE POTTS MODEL

By

Ibrahim Fatkullin

A Thesis Submitted to the Graduate  
Faculty of Rensselaer Polytechnic Institute  
in Partial Fulfillment of the  
Requirements for the Degree of  
DOCTOR OF PHILOSOPHY  
Major Subject: Mathematics

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Rensselaer Polytechnic Institute  
Troy, New York

July 2002  
(For Graduation August 2002)

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## Abstract

This work is devoted to the statistical description of certain stochastic partial differential equations (PDEs) which exhibit the so-called **phase separation** dynamics. In particular we consider the randomly perturbed scalar Ginzburg-Landau (or Allen-Cahn) equation (1.1) and the Cahn-Hilliard equation (1.2). Deterministic dynamics of these systems in certain asymptotic limits is quickly attracted to the so-called **slow manifold** — a set of functions assuming a discrete set of values (phases) almost everywhere, and further on proceeds restricted to this set. We develop a formalism which allows the analysis of the asymptotic dynamics in both the deterministic and stochastic settings via a restriction of the full gradient flow to the slow manifold.

The second problem that we study is the influence of small stochastic perturbations on the reduced dynamics of the aforementioned systems. It turns out that in the proper asymptotic limit the deterministic dynamics of one-dimensional systems is totally dominated by the noise, and reduces to the dynamics of an ensemble of particles which undergo Brownian motions and interact by collision. We also discuss the **nucleation** phenomenon which consists of the creation of new domains induced by the large fluctuations of the stochastic forcing. We complete the PDE aspect of this work by summarizing these ideas and establishing the connection with the so-called **Potts model with voters** dynamics, to which we devote the rest of our studies.

Our interest lies in the understanding of the **coarsening** phenomenon. It appears in connection with the question of the general structure of solutions in spatially extended systems, i. e., in the situation when there exists a large number of **domains** (connected regions of a certain phase), and concerns the distribution of domain sizes and their elimination in the process of evolution.

The Potts model with voters dynamics is a stochastic process on lattice **spin** systems. It describes the switching of the spin values at random times to the values of their immediate neighbors. The continuous limit of the Potts model is directly related to the reduced dynamics of the Ginzburg-Landau equation and therefore the analysis of the statistical properties of the former provides understanding of the coarsening phenomena in original PDEs. We begin with the introduction of some basic facts concerning one-dimensional spin lattices and comparison of several different ways to obtain their probabilistic description, e. g., by means of **correlation functions** and **domain-length densities**. Next we derive evolution equations for these quantities induced by the voters dynamics and analyze their continuous limits. We find that an infinite hierarchy of coupled equations is necessary to provide the complete description and discuss possible **decouplings** and **closures**.

## CHAPTER 1

### Introduction

One of the central topics in the current studies of non-equilibrium dynamics is the problem of domain formation and evolution in magnetic or other systems undergoing phase separation. The mathematical treatment of these problems follows several different approaches. One such approach is to consider a partial differential equation, derived from the physical model, which describes the evolution of some order parameter field – a real function  $u(\mathbf{x}, t)$  of the spatial and temporal variables. The most widely used models include the so-called scalar Ginzburg-Landau, or Allen-Cahn equation

$$\partial_t u = \delta \Delta u - \frac{1}{\delta} V'(u), \quad V(u) = \frac{1}{4}(1 - u^2)^2, \quad (1.1)$$

and the Cahn-Hilliard equation

$$\partial_t u = -\Delta(\delta \Delta u - \frac{1}{\delta} V'(u)). \quad (1.2)$$

These equations are solved in some domain  $\Omega \in \mathbb{R}^k$  with suitable boundary conditions. For the purposes of this work, we will generally assume periodic boundary conditions (possibly considering the limit as the period goes to infinity). The function  $V(u)$  is called the potential. In particular we call the potential defined in (1.1) the Ginzburg-Landau potential. In case  $V(u)$  is different, we call the corresponding equations Ginzburg-Landau or Cahn-Hilliard-type equations. The potential will be always assumed to have two or more minima.

Our particular interest lies in the analysis of the asymptotic ( $\delta \rightarrow 0$ ) behavior of systems of the type (1.1) or (1.2) and their small stochastic perturbations. The goal is to reach understanding of the statistical properties of the solutions in this asymptotic limit.

The major similarity between the two aforementioned equations is the existence of a very specific reduced asymptotic (as  $\delta \rightarrow 0$ ) dynamics, and the major difference is that the Cahn-Hilliard equation conserves the total integral of the field  $\hat{\mathcal{F}}[u] = \int u(\mathbf{x}) d\mathbf{x}$ . Let us notice that the both systems are gradient, i. e., may be represented in the form<sup>1</sup>

$$\partial_t u = -D_u \mathcal{E}[u], \quad (1.3)$$

where  $\mathcal{E}[u]$  is the energy functional and  $D_u$  denotes the variational derivative. Thus for the Allen-Cahn equation

$$\mathcal{E}[u] = \int_{\Omega} \left[ \frac{\delta}{2} |\nabla u|^2 + \frac{1}{\delta} V(u) \right] d\mathbf{x}. \quad (1.4)$$

---

<sup>1</sup>Later on we will discuss a more general geometric formulation of gradients flows.

The Cahn-Hilliard equation (1.2) can be written in the form (1.3) after a change of variables, in which case (1.2) is equivalent to

$$\partial_t \mathbf{v} = -\mathbf{D}_{\mathbf{v}}\mathcal{E}[\nabla \cdot \mathbf{v}], \quad u(\mathbf{x}, t) = \nabla \cdot \mathbf{v}(\mathbf{x}, t). \quad (1.5)$$

Notice that these systems dissipate energy, indeed  $\partial_t \mathcal{E} = -\|\mathbf{D}_{u(\mathbf{x})}\mathcal{E}[u]\|^2$  and therefore the energy of the system is a non-increasing quantity <sup>2</sup>.

**Random perturbations.** During the derivations leading to the field equations, mentioned earlier, various approximations are necessarily made and in order to account for the neglected degrees of freedom, it is common to introduce additional stochastic driving into the deterministic model. The limit when the strength of the noise diminishes is generally referred to as the zero-temperature dynamics and is often assumed to be properly described by the deterministic equations. This statement is, however, not generally correct and noise effects, however small, may greatly affect dynamics of the system. This is especially true if the deterministic dynamics becomes **frozen**, i. e., attracted to the **meta-stable** or **quasi-stable** states, where subsequent motion is almost non-existent.

**Spin systems and Potts models.** An alternative approach is based on the modelling of the magnetic system by a **spin lattice** with appropriate interaction (e. g., **Glauber** or **voters** dynamics). Such models are often intrinsically stochastic, and the aforementioned continuous field equations may be obtained by taking scaling limits of the spin systems. There exist different classes of problems related to spin systems, e. g., the problem of **aging** and **persistence** studied in a series of works by L. R. Fontes and M. Isopi and C. M. Newman and D. L. Stein [19], or the problem of domain-length distribution studied by B. Derrida and R. Zeutak [13], P. A. Alemany, D. ben-Avraham and T. Masser [1], [28], E. Ben-Naim and P. L. Krapivsky [3], [26].

In the current work, we consider one-dimensional Potts models from the point of view of domain-length distribution and establish their connection with the dynamics of the Ginzburg-Landau equation. We provide a systematic derivation of the hierarchies of equations for domain-length probability densities and discuss their closures.

We restrict our attention to the domain-length probability densities because they provide the most complete information about the system whereas all the other quantities can be easily obtained from the knowledge of them.

**Coarsening.** In the study of interface dynamics one usually considers two complementary regimes that depend on the complexity of the initial conditions. The first regime includes a small number of interfaces. Detailed questions of formation and propagation of a single interface or the interaction among the small number of interfaces are studied in this regime. The second, ‘thermodynamic limit,’ regime includes vast numbers of interfaces. In this regime one studies statistical properties

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<sup>2</sup>The corresponding law for the Cahn-Hilliard equation reads  $\partial_t \mathcal{E} = -\|\mathbf{D}_{\mathbf{v}(\mathbf{x})}\mathcal{E}[\nabla \cdot \mathbf{v}]\|^2 = -\|\nabla \mathbf{D}_{u(\mathbf{x})}\mathcal{E}[u]\|^2$ .



of domain-length distributions, correlation functions, etc. The dynamics of such large systems exhibits coarsening during which domains of different phases increase in size, whereas the general statistical structure, after a proper rescaling, remains the same.

We begin by considering small systems in order to understand their asymptotic dynamics. However, it will become clear that the interactions appearing in the asymptotic limit (as  $\delta \rightarrow 0$ ) are local (which is especially true in the case of one dimensional stochastic systems), and the transition to large systems is effortless. The second part of this work is solely devoted to large systems and their statistical description.

The problem of coarsening for the deterministic one-dimensional Allen-Cahn (or scalar Ginzburg-Landau) equation has been studied by J. Carr and R. L. Pego [10] and also by J.-P. Eckmann and J. Rougemont [15]. Studies of coarsening dynamics for the Cahn-Hilliard equation were undertaken by C. L. Emmott and A. J. Bray [16].

Thesis outline. The organization of the thesis is as follows. Chapter 2 is concerned with the asymptotic limit of Ginzburg-Landau-type equations. We introduce a formalism suitable for analysis of both deterministic and stochastic systems. We apply this formalism to several examples and review the reduction of the PDE dynamics to the motion by mean curvature in two and more dimensions, or to the ensemble of interacting particles in the one-dimensional case.

In Chapter 3 we consider the influence of stochastic forcing on the dynamics on the slow manifold. We demonstrate that, in the limit of small noise, the dynamics is still restricted to the slow manifold, but appears stochastic rather than deterministic. Moreover, for one-dimensional systems in the appropriate limit, the deterministic motion is totally dominated by the stochastic motion, and the whole problem becomes equivalent to a diffusion-annihilation process. The nucleation phenomenon is also studied as a necessary ingredient to achieve the statistical equilibrium state.

Chapter 4 presents a detailed theory used for statistical analysis of ensembles of diffusing particles with various interactions (Potts models with voters dynamics) based on domain-length probability densities. As is shown in Chapter 3, the two-state Potts model is intimately related to the dynamics of Allen-Cahn-type stochastic partial differential equations, and therefore is essential for the understanding of the latter. Moreover, we do not limit ourselves to the diffusion-annihilation process only, but rather analyze different Potts models in a unified framework. In our discussion, we first consider discrete spin-lattice systems with voters dynamics and then take a scaling limit to obtain the corresponding continuous systems.

## CHAPTER 2

### Asymptotic behavior of certain gradient systems

#### 2.1 Motivation and general setting

Our first goal is to develop a formalism which will allow us to consider both deterministic and stochastically perturbed asymptotic dynamics of gradient systems of the type (1.1) or (1.2) in a unified framework. We are interested in the limit  $\delta \rightarrow 0$  with initial conditions that have energy (1.4) of  $\mathcal{O}(1)$ . Such a limit corresponds to the **phase separation** dynamics —  $u(x)$  is forced to assume values close to those from the set  $\{v : V(v) = 0\}$  everywhere, except on boundary layers, which comprise a set of measure of  $\mathcal{O}(\delta)$ . This follows directly from (1.4). In particular, in the one-dimensional case, these boundary layers can be locally approximated by the travelling<sup>3</sup> wave solutions of (1.1). In higher dimensions, the boundary layers generally form curves (or surfaces) and locally the field in the normal direction has the same form as in the one-dimensional case.

Piecewise continuous functions of the form  $u(\mathbf{x}) \in \{v : V(v) = 0\}$  for all  $\mathbf{x}$  except a set of measure 0 form the so-called **slow manifold**, and in the asymptotic limit, the dynamics is restricted to this manifold. If the system starts away from this manifold it will decay to it in a very short,  $\mathcal{O}(\delta)$ , time, whereas the evolution along the slow manifold is either exponentially slow in  $\delta$  (in the one-dimensional case), or of  $\mathcal{O}(1/\delta)$  in higher dimensional systems.

For example, the functions mentioned above are uniquely determined by the specification of the domain boundary, which is assumed to be the 0-level set of some function  $\ell(\mathbf{x})$ . In this case  $\ell$  is exactly the local coordinate on the slow manifold. However, we also need information concerning the structure of the boundary layers to be able to identify the tangent space of the slow manifold.

The central idea in our analysis of the slow dynamics consists of recasting the original equations in terms of the local coordinates of the slow manifold via restricting the metric tensor that defines the gradient flow to the cotangent space  $T^*\mathcal{M}_s \otimes T^*\mathcal{M}_s$  of the slow manifold alone. This procedure may in fact be performed for any submanifold  $\mathcal{M}'$  of the full function space  $\mathcal{M}$  and produces a new gradient system which is equivalent to the original one constrained to  $\mathcal{M}'$ . The reason for the application of this restriction to the slow manifold  $\mathcal{M}_s$  is that the dynamics is in any case restricted to  $\mathcal{M}_s$  and therefore making this explicit provides a considerable reduction in the number of degrees of freedom for which we have to account.

Remark on the slow manifold. The slow manifold as described above is strictly speaking a set of functions which are very close to the solution of the corresponding gradient system at all times except for a certain discrete set  $\{\tau_i\}$ . At times  $t$  such that  $|t - \tau_i| = \mathcal{O}(\delta)$ , the approximations

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<sup>3</sup>In fact, for the Ginzburg-Landau potential, these travelling waves are pinned.

which we make become invalid and the dynamics is in fact very fast, e. g., proceeds on an  $\mathcal{O}(1/\delta)$  time scale. This phenomenon occurs, for example, at the times of kink collision in the one-dimensional Ginzburg-Landau equation<sup>4</sup>. Nevertheless right after such a ‘burst’ of activity is over, the solution becomes quasi-stationary and its evolution proceeds on a much longer time-scale and can be described in terms of the slow manifold again. So, in fact, the slow manifold is an entire collection of manifolds and the solution occasionally jumps from to another at times  $\tau_i$ .

## 2.2 Identification of the slow manifold

We turn to the problem of how to identify the slow manifold. This is done by an asymptotic expansion of the original equations as  $\delta \rightarrow 0$  with the goal of revealing the set of functions stationary on the fast time scales. Let us notice that the fact that we only want to obtain solutions that are stationary on the  $\mathcal{O}(1)$  time scale significantly decreases the complexity of the asymptotic analysis. We will consider the multi-dimensional Ginzburg-Landau equation to illustrate the basic ideas and later on, when dealing with more general systems, will briefly comment on their differences and similarities.

### 2.2.1 Slow manifold in several spatial dimensions

Before we begin our analysis, let us mention that this question has been well-studied, and, therefore, we will only give a brief summary of the existing results. It is known that, in the asymptotic limit, the energy functional (1.4) converges to a quantity proportional to the perimeter of the boundary interface

$$\mathcal{E}[u] \rightarrow \mathcal{E}_\ell = \frac{2\sqrt{2}}{3} \oint_{\ell(\mathbf{x})=0} dl, \quad (2.1)$$

where the integral is taken over the 0-level set of some function  $\ell(\mathbf{x})$ , on which the boundary interface forms ( $dl$  is a surface element). The solution of the gradient flow (1.1) converges to the gradient flow<sup>5</sup> on the local minimizers of the energy  $\mathcal{E}$ . These minimizers have been studied by R. V. Kohn and P. Sternberg [25], [38]. Also H. M. Soner undertook an extensive study of this topic in the context of weak solutions [36], [37]. We will first undertake a formal asymptotic analysis of (1.1) in the spirit of the treatment by J. Rubinstein, P. Sternberg and J. B. Keller [33]. When it becomes clear which functions form the slow manifold, we will diverge from their method, and will instead use the ideas discussed in Section 2.3 to analyze the dynamics.

Let us consider the Allen-Cahn equation

$$\partial_t u = \delta \Delta u - \frac{1}{\delta} V'(u). \quad (2.2)$$

---

<sup>4</sup>The maximum principle does not allow merging of the domains in higher dimensions (at least in deterministic systems). However, in this case, a similar phenomenon occurs when the entire domains vanish during the motion by mean curvature.

<sup>5</sup>Evolution of course proceeds on an  $\mathcal{O}(\delta)$  time scale.

Introducing the new time variable  $\tau = t/\delta$  and expanding

$$u(\mathbf{x}, t) = v^{(0)}(\mathbf{x}, \tau) + \delta^2 v^{(1)}(\mathbf{x}, \tau) + \mathcal{O}(\delta^4) \quad (2.3)$$

we immediately find

$$\partial_\tau v^{(0)} = -V'(v^{(0)}), \quad (2.4)$$

i. e., the evolution on the  $\mathcal{O}(1/\delta)$  time scale obeys an ordinary differential equation in which  $\mathbf{x}$  is merely a parameter. We see that as  $\tau \rightarrow \infty$ ,  $v^{(0)}$  converges to the local minima  $\{v_i\}$  of the potential  $V$ , and the entire domain  $\Omega$  is thus subdivided into smaller subdomains on which  $u(\mathbf{x})$  assumes the values from  $\{v_i\}$ . The asymptotic expansion (2.3) of course loses its validity near the boundaries of these subdomains (which we assume to be the 0-level sets of some function  $\ell(\mathbf{x})$ ) and we have to introduce a new expansion

$$u(\mathbf{x}, t) = u^{(0)}(y, \mathbf{x}, \tau, t) + \delta u^{(1)}(y, \mathbf{x}, \tau, t) + \mathcal{O}(\delta^2), \quad y = \frac{1}{\delta} \ell(\mathbf{x}, t). \quad (2.5)$$

The equation for the first-order terms in this expansion reads

$$u_\tau^{(0)} + \ell_t u_y^{(0)} - |\nabla_{\mathbf{x}} \ell|^2 u_{yy}^{(0)} + V'(u^{(0)}) = 0. \quad (2.6)$$

Assuming that  $u^{(0)}$  tends to a travelling wave  $u^{(0)}(y, \mathbf{x}, \tau, t) \approx w(y - c\tau, \mathbf{x}, t, \eta)$  as  $\tau \rightarrow \infty$  and using (2.6), we obtain

$$-|\nabla_{\mathbf{x}} \ell|^2 w_{yy} + (\ell_t - c)w_y + V'(w) = 0. \quad (2.7)$$

If the boundary separates the phases  $v_i$  and  $v_j$  (which are the limiting values of  $u$  on different sides of the front as  $y \rightarrow \pm\infty$ ), then multiplying the last expression by  $w_y$  and integrating over  $y$ , we find

$$\ell_t - c = -[V] \left[ \int_{\mathbf{R}} (w_y)^2 dy \right]^{-1}, \quad [V] = V(v_j) - V(v_i). \quad (2.8)$$

For the Ginzburg-Landau potential,  $V(u) = \frac{1}{4}(1 - u^2)^2$ , and therefore  $[V] = 0$ . Equation (2.8) forces  $\ell_t = c$ , and consequently the fronts are stationary on the time scale  $t$ . The appropriate solution to (2.7) thus reads

$$w(y) = \tanh(y/(\sqrt{2}|\nabla_{\mathbf{x}} \ell|)), \quad (2.9)$$

and defines the profile of the boundary interface. We have thus concluded the identification of the slow manifold. For the Ginzburg-Landau potential, the latter is the set of functions assuming  $\pm 1$  everywhere except on the level sets of  $\ell(\mathbf{x})$ , which prescribe the location of the boundary layers. The local shape of these functions near the interface is given by equation (2.9).

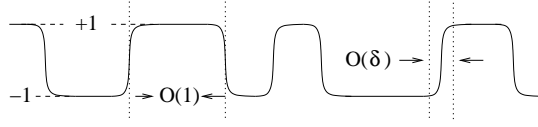


Figure 2.1: Schematic representation of multi-kink solutions

## 2.2.2 Slow manifold in one spatial dimension and reduction to a system of particles

We begin again with the asymptotic analysis of

$$\partial_t u = \delta \partial_{xx}^2 u - \frac{1}{\delta} V'(u). \quad (2.10)$$

As in higher dimensions, the asymptotic solutions assume the values  $v_i$  that provide the minima for the potential  $V(u)$  everywhere except in thin layers of  $\mathcal{O}(\delta)$ . We will assume that  $V(v_i) = 0$  so that all the kinks are stationary. In particular, for the Ginzburg-Landau potential, the explicit form of the boundary layers is  $u^\pm = \pm \tanh((x - \zeta)/\sqrt{2}\delta)$ , where  $\zeta$  is the location of such a layer.

One can construct the composite, multi-kink solutions connecting the stable phases  $u = v_i$  by using these boundary layers. Any such solution is defined by specifying the locations of the kinks and the stable phases which they connect. This will be denoted in the following manner:

$$u_\zeta(x) = u_j^i(x - \zeta_1) \bullet u_k^j(x - \zeta_2) \bullet \dots, \quad (2.11)$$

which means that there is a kink located at  $\zeta_1$ , connecting phases  $v_i$  and  $v_j$ , followed by a kink at  $\zeta_2$  connecting  $v_j$  with  $v_k$ , and so on. Figure 2.1 presents a general structure of multi-kink solutions for the Ginzburg-Landau equation.

In the limit as  $\delta \rightarrow 0$ , these solutions degenerate into step functions and form the slow manifold. The motion on the slow manifold (which in the case of an  $N$ -kink solution has dimension  $N$ ) can be completely described by the shift of the kink locations  $\zeta_i$ , which play the role of the local coordinates. Therefore, we associate this dynamics with that of a system of particles. The correspondence between the boundary layers and particles is seen in the following manner: Suppose  $V$  has minima which follow in the sequence  $v_1 < \dots < v_n$ . Every boundary layer is a heteroclinic orbit of the Hamiltonian system obtained from (2.10) by considering stationary solutions. Such a boundary layer connects two nearest minima and therefore we assign a ‘color’ to it, which is the index  $k$  of the first minimum in the sequence. We then call it a kink or an anti-kink depending on whether it connects  $v_k$  and  $v_{k+1}$  or, conversely,  $v_{k+1}$  and  $v_k$ . Thus, we set a correspondence between the field  $u(x)$  and a set of kinks on the line by specifying the locations and colors of the kinks.

In the one-dimensional system the 0-level sets of  $\ell$  are just the points  $\zeta_i$ . Their locations provide the local coordinates on the slow manifold.

The evolution of this system of particles obeys certain laws which we will derive shortly. If ever a kink and an anti-kink of the same color collide, they annihilate. On the other hand, kinks of different colors may neither annihilate nor pass through each other<sup>6</sup>. There exists such an evolution  $\zeta(t)$  for the particles that<sup>7</sup>

$$\|u(x, t) - u_j^i(x - \zeta_1(t)) \bullet u_k^j(x - \zeta_2(t)) \bullet \dots\| = \mathcal{O}(\delta). \quad (2.12)$$

For Ginzburg-Landau-type equations, this evolution is given by equation (2.38) below. The number of particles is of course not preserved, and there exists a sequence of times  $\{\tau_1, \dots, \tau_n\}$  at which collisions occur, particles annihilate and should be relabelled. In fact a stronger statement is true. The  $\mathcal{O}(\delta)$  mismatch between the actual solution and a multi-kink approximation only appears at times up to  $\mathcal{O}(\delta)$  close to these collision times  $\tau_i$ . At all other times these two functions are exponentially  $\mathcal{O}(\exp\{-\lambda_{\min}/\delta\})$  close to one another, where  $\lambda_{\min}$  is the smallest distance between the kinks. This estimate, however, obviously loses its sense in the situation when the size of the spatial domain for  $u(x)$  grows to infinity.

### 2.3 Geometric approach and restriction of the dynamics

After the identification of the slow manifold has been completed, and we have understood that it consists of functions defined by the level sets of  $\ell(\mathbf{x})$ , we can take the latter as a convenient parametrization and rewrite the original equations in terms of  $\ell$  rather than  $u$ .

Here we describe the techniques necessary for deriving equations on the slow manifold.

We use a geometric interpretation of gradient systems and describe how a gradient flow constrained on a submanifold is obtained via a restriction of the metric tensor.

Let us begin with introducing some convenient (although slightly formal) notation borrowed from geometry. First of all, gradient systems of the form (1.3) should in fact be written as equations for vector fields in the following manner. Let  $\mathcal{M}$  designate a manifold of functions acting from  $\Omega$  to  $\mathbb{R}$ . Let  $\hat{\mathbf{g}} \in \mathcal{T}^*\mathcal{M} \otimes \mathcal{T}^*\mathcal{M}$  be a metric tensor (which in this work we assume to be symmetric)

$$\hat{\mathbf{g}} = \int d\mathbf{x} \int d\mathbf{y} g(\mathbf{x}, \mathbf{y}) d\mathbf{u}(\mathbf{x}) \otimes d\mathbf{u}(\mathbf{y}), \quad (2.13)$$

where  $d\mathbf{u}(\mathbf{x})$  are the basis 1-forms dual to the bases  $\partial_{u(\mathbf{x})}$  in the tangent space  $\mathcal{T}\mathcal{M}$ , i. e.,

$$d\mathbf{u}(\mathbf{x}) \partial_{u(\mathbf{y})} = \delta(\mathbf{x} - \mathbf{y}). \quad (2.14)$$

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<sup>6</sup>In fact, the kinks of different colors repulse each other so that they never collide in the deterministic setting.

<sup>7</sup>The norm is  $\mathbb{L}^2$  in  $x$  and  $t$ .

The gradient  $D_u \mathcal{E}$  should be written as a 1-form

$$d\mathcal{E} = \int d\mathbf{x} D_{u(\mathbf{x})} \mathcal{E}[u] d\mathbf{u}(\mathbf{x}). \quad (2.15)$$

The gradient vector field  $\partial_t = \int d\mathbf{x} u_t(\mathbf{x}) \partial_{u(\mathbf{x})}$  is defined by the equation which in the covariant form reads

$$\hat{\mathbf{g}} \partial_t = -d\mathcal{E}, \quad (2.16)$$

or componentwise, using the four last equations

$$\int g(\mathbf{x}, \mathbf{y}) u_t(\mathbf{y}) d\mathbf{y} = -D_{u(\mathbf{x})} \mathcal{E}[u] \quad (2.17)$$

which can also be written in the ‘regular’ form by inverting the operator on the left-hand side.

**Restriction of the dynamics.** The fact that the dynamics is limited to the slow manifold  $\mathcal{M}_s$  can be explicitly formulated by restricting the vector and covector fields in (2.16) to the tangent,  $\mathcal{TM}_s$ , and cotangent,  $\mathcal{T}^*\mathcal{M}_s$ , spaces of the slow manifold alone. This is done by a simple change of variables, chosen via a convenient parametrization  $\ell(\mathbf{x})$  on  $\mathcal{M}_s$

$$\partial_{u(\mathbf{x})} = \int d\mathbf{y} D_{u(\mathbf{x})} \ell(\mathbf{y}) \partial_{\ell(\mathbf{y})}, \quad d\mathbf{u}(\mathbf{x}) = \int d\mathbf{y} D_{\ell(\mathbf{y})} u(\mathbf{x}) d\ell(\mathbf{y}) \quad (2.18)$$

and therefore<sup>8</sup>

$$\begin{aligned} \hat{\mathbf{g}}_s &= \int d\mathbf{x} \int d\mathbf{y} g_s(\mathbf{x}, \mathbf{y}) d\ell(\mathbf{x}) \otimes d\ell(\mathbf{y}), \\ g_s(\mathbf{x}, \mathbf{y}) &= \int d\mathbf{x}' \int d\mathbf{y}' g(\mathbf{x}', \mathbf{y}') D_{\ell(\mathbf{x})} u(\mathbf{x}') D_{\ell(\mathbf{y})} u(\mathbf{y}'). \end{aligned} \quad (2.19)$$

Notice that now  $\partial_{v(\mathbf{x})}$  and  $d\mathbf{v}(\mathbf{x})$  belong to  $\mathcal{TM}_s$  and  $\mathcal{T}^*\mathcal{M}_s$ , respectively, and of course the equation for  $\partial_t$  has the same form (2.16) with  $\hat{\mathbf{g}}$  replaced by  $\hat{\mathbf{g}}_s$ , or componentwise

$$\int g_s(\mathbf{x}, \mathbf{y}) \ell_t(\mathbf{y}) d\mathbf{y} = -D_{\ell(\mathbf{x})} \mathcal{E}[v]. \quad (2.20)$$

**Metric of the inverse Laplacian.** For ‘regular’ gradient systems of the form (1.3) the metric tensor is just

$$\hat{\mathbf{g}} = \int d\mathbf{x} \int d\mathbf{y} \delta(\mathbf{x} - \mathbf{y}) d\mathbf{u}(\mathbf{x}) \otimes d\mathbf{u}(\mathbf{y}). \quad (2.21)$$

A complication arises when one tries to deal with the Cahn-Hilliard-type equations (1.2) or more generally with equations of the form

$$\partial_t u = -\hat{A} D_u \mathcal{E}, \quad (2.22)$$

---

<sup>8</sup>This change of variables is an actual restriction if only  $\mathcal{TM}_s$  is a proper subspace of  $\mathcal{TM}$ , otherwise it is just a change of local parametrization.

where  $\hat{A}$  is some symmetric degenerate positive-semidefinite operator. In order to write such a system in the general gradient form (2.16), i. e., to construct the proper metric tensor, one basically has to obtain  $\hat{A}^{-1/2}$ , whereas  $\hat{A}$  is not invertible. For example, for the regular Cahn-Hilliard equation, in which  $\hat{A}$  is the Laplacian, the metric tensor formally reads

$$\hat{\mathbf{g}} = \int d\mathbf{x} \int d\mathbf{y} \nabla_{\mathbf{x}}^{-1} \cdot \nabla_{\mathbf{y}}^{-1} \delta(\mathbf{x} - \mathbf{y}) d\mathbf{u}(\mathbf{x}) \otimes d\mathbf{u}(\mathbf{y}), \quad (2.23)$$

which is not properly defined.

In order to deal with this problem let us first notice the fact that the degeneracy of  $\hat{A}$  leads to a number of conservation laws for the dynamics. Let us designate the corresponding conserved quantities by  $\hat{\mathcal{F}}_i$ . The kernel of  $\hat{A}$  is then spanned by  $D_{u(\mathbf{x})}\hat{\mathcal{F}}_i[u]$  which is exactly the subspace where we fail to define the metric tensor. On the other hand, knowing that evolution is ‘orthogonal’ to this subspace, all we have to do in order to obtain a well-defined metric tensor is to reduce the tangent space to the intersection of the kernels<sup>9</sup> of the gradients  $\int d\mathbf{x} D_{u(\mathbf{x})}\hat{\mathcal{F}}_i[u] d\mathbf{u}(\mathbf{x})$  of the conserved quantities. Returning back to the Cahn-Hilliard equation where  $\hat{A}$  is the Laplacian, we notice that the kernel consists of constant functions<sup>10</sup>, and therefore the tangent space  $\mathcal{TM}$  is reduced to the vectors  $\int d\mathbf{x} f(\mathbf{x}) \partial_{u(\mathbf{x})}$  such that  $\int f(\mathbf{x}) d\mathbf{x} = 0$ . The operator  $\nabla^{-1}$  in (2.23) is properly defined on such functions (e. g., in their Fourier series representation).

Technically, when writing equations on the slow manifold, one can immediately choose a parametrization which leaves out the degenerate directions. However, it is often more convenient to use a different parametrization and projection operators

$$\begin{aligned} \hat{\mathbf{P}} &= \int d\mathbf{x} \int d\mathbf{y} \left[ \delta(\mathbf{x} - \mathbf{y}) - \frac{1}{\mu} D_{\ell(\mathbf{y})}\hat{\mathcal{F}}[\ell] \right] \partial_{\ell(\mathbf{x})} \otimes d\ell(\mathbf{y}), \\ \mu &= \int D_{\ell(\mathbf{x})}\hat{\mathcal{F}}[\ell] d\mathbf{x}. \end{aligned} \quad (2.24)$$

to enforce the dynamics on the proper subspace. In this case, the metric tensor and the 1-form of the energy should be transformed into  $\hat{\mathbf{P}} \hat{\mathbf{g}}_s \hat{\mathbf{P}}$  and  $d\mathcal{E} \hat{\mathbf{P}}$ , respectively. This technique will be illustrated later on in Section 2.4 when we discuss the constrained Allen-Cahn and Cahn-Hilliard equations.

## 2.4 Examples

Here we consider several problems which will employ all the ideas discussed earlier. As an example of multi-dimensional systems we analyze the Ginzburg-Landau equation and derive equations for the motion by mean curvature of the boundary layers. Let us mention some of the

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<sup>9</sup>Notice, that we here use the kernel of the form which is orthogonal (in the sense of duality) to the kernel of the operator  $\hat{A}$  mentioned before.

<sup>10</sup>That is of course for periodic domains, otherwise there also exist nontrivial solutions of Laplace’s equation with proper boundary conditions.



extensive literature on the subject the reduction of PDE dynamics to different geometric evolutions. L. C. Evans, H. M. Soner and P. E. Souganidis considered generalizations of the motion by mean curvature in [17]. A detailed analysis of different surface evolution equations based on the level set methods can be found in the book by Y. Giga [23].

We also consider several systems in one dimension. The Cahn-Hilliard was studied by R. L. Pego [30] in a similar style based on the asymptotic expansions. J. Rougemont [32] considered the problem of droplet evaporation in the two-dimensional Ginzburg-Landau equation.

#### 2.4.1 Multi-dimensional Ginzburg-Landau dynamics

Let us follow the treatment described in Section 2.3 to derive the asymptotic dynamics for the Ginzburg-Landau equation. We parametrize the slow manifold by  $\ell(\mathbf{x})$ , i. e., it consists of functions of the form  $u(\mathbf{x}) = \tanh(\ell(\mathbf{x})/(\sqrt{2}\delta|\nabla\ell|))$ . First we calculate the metric tensor in the  $\ell$ -parametrization (recall that in the  $u$ -parametrization it has the form (2.21)). The variational derivatives used in (2.19) are easy to calculate

$$D_{\ell(\mathbf{y})}u(\mathbf{x}) = \frac{1}{\sqrt{2}\delta|\nabla\ell(\mathbf{x})|} \cosh^{-2}\left(\frac{\ell(\mathbf{x})}{\sqrt{2}\delta|\nabla\ell(\mathbf{x})|}\right) \times \left[ \delta(\mathbf{x} - \mathbf{y}) + \frac{\ell(\mathbf{x})}{|\nabla\ell(\mathbf{x})|^2} \nabla\ell \cdot \nabla_{\mathbf{y}} \delta(\mathbf{x} - \mathbf{y}) \right], \quad (2.25)$$

and therefore by substituting the last expression into (2.19) we obtain the matrix of the metric tensor<sup>11</sup>

$$g_s(\mathbf{x}, \mathbf{y}) = \frac{1}{2\delta^2|\nabla\ell|^2} \cosh^{-4}\left(\frac{\ell(\mathbf{x})}{\sqrt{2}\delta|\nabla\ell|}\right) \delta(\mathbf{x} - \mathbf{y}) + \mathcal{O}(\ell). \quad (2.26)$$

Equations for the vector fields contain integration of  $g_s$  over the entire space, and it is not hard to see that since the  $\cosh^{-4}$  prefactor converges to a  $\delta$ -function localized on the 0-level set of  $\ell$ , as  $\delta \rightarrow 0$ , such integrals are reduced to integrals over the the level set  $\ell(\mathbf{x}) = 0$ . In this sense

$$g_s(\mathbf{x}, \mathbf{y}) \rightarrow \tilde{g}_s(\mathbf{x}, \mathbf{y}) = \frac{2\sqrt{2}}{3\delta|\nabla\ell|^2} \delta(\mathbf{x} - \mathbf{y}). \quad (2.27)$$

The Ginzburg-Landau energy functional on the slow manifold reads

$$\mathcal{E}[v] = \int \frac{1}{2\delta} \cosh^{-4}(\ell(\mathbf{x})/(\sqrt{2}\delta|\nabla\ell|)) \left[ 1 + \mathcal{O}(\ell) \right] d\mathbf{x}, \quad (2.28)$$

which, as  $\delta \rightarrow 0$ , clearly converges to

$$\mathcal{E}[v] \rightarrow \mathcal{E}_\ell = \frac{2\sqrt{2}}{3} \oint_{\ell(\mathbf{x})=0} dl. \quad (2.29)$$

---

<sup>11</sup>Here and in the expression (2.28) for the energy we use notation  $\mathcal{O}(\ell)$  to denote those terms which only contribute to higher orders in  $\delta$  after integration over the entire space.

Equation (2.16) now reads

$$\oint_{\ell(\mathbf{x})=0} d\ell \oint_{\ell(\mathbf{y})=0} d\ell' \tilde{g}_s(\mathbf{x}, \mathbf{y}) \partial_t \ell(\mathbf{y}) \boldsymbol{\partial}_{\ell(\mathbf{x})} = \oint_{\ell(\mathbf{x})=0} d\ell \mathbf{D}_{\ell(\mathbf{x})} \mathcal{E}[\ell] \boldsymbol{\partial}_{\ell(\mathbf{x})}. \quad (2.30)$$

Using (2.27) and (2.29) we can write the asymptotic equation for the gradient vector field as

$$\partial_t \ell(\mathbf{x}) = -\frac{3\sqrt{2}\delta}{4} |\nabla \ell(\mathbf{x})|^2 \mathbf{D}_{\ell(\mathbf{x})} \mathcal{E}_\ell, \quad (2.31)$$

which immediately yields

$$\partial_t \ell = \delta |\nabla \ell| \left[ \Delta \ell - \frac{\nabla \ell \cdot \nabla |\nabla \ell|}{|\nabla \ell|} \right] \quad (2.32)$$

— the equation for the motion by mean curvature  $\kappa_\ell$  of the level sets of  $\ell$ . This can be easily rewritten for some particular level set of  $\ell$ , yielding the equation for its normal velocity  $v(\mathbf{x})$

$$v(\mathbf{x}) = \delta \kappa_\ell(\mathbf{x}), \quad \kappa_\ell = \nabla \cdot \left[ \frac{\nabla \ell}{|\nabla \ell|} \right]. \quad (2.33)$$

#### 2.4.2 One-dimensional systems

Dynamics in one spatial dimension is significantly different from that considered before. There is no curvature of the interfaces and the level sets of  $\ell(x)$  are just the sets of points around which the transition layers are localized. Therefore, it is more convenient to parametrize the slow manifold by simply specifying the zeros  $\zeta_i$  of the field  $u(x)$ . One can find the treatment based on the asymptotic analysis of Ginzburg-Landau-type equations with multi-well potentials  $V(u)$  in the works by J. Rubinstein, P. Sternberg and J. B. Keller, e. g. [34]. The problem of the bubble interaction in the Cahn-Hilliard equation was studied by H. Calisto, M. Clerc, R. Rojas and E. Tirapegui [9].

**Ginzburg-Landau-type equations.** Let us first notice that since the slow manifold is now finite-dimensional formulas (2.18) should read

$$\boldsymbol{\partial}_{u_\zeta(x)} = \sum_i \frac{\phi_i(x)}{\|\phi_i\|^2} \boldsymbol{\partial}_{\zeta_i}, \quad \mathbf{d}u_\zeta(x) = \sum_i \phi_i(x) \mathbf{d}\zeta_i \quad (2.34)$$

and in other similar formulas integration is simply reduced to the sum over the kinks ( $i = 1 \dots N$ ). In the last expression, we have used are the functions  $\phi_i(x) = \partial_{\zeta_i} u_\zeta(x)$  (analogues of  $\mathbf{D}_{\ell(\mathbf{y})} u(\mathbf{x})$  in the multi-dimensional systems), e. g., for the Ginzburg-Landau equation

$$\phi_i(x) = \frac{(-1)^i}{\sqrt{2\delta}} \cosh^{-2} \left( \frac{x - \zeta_i}{\sqrt{2\delta}} \right), \quad \|\phi_i\| = \left[ \frac{2\sqrt{2}}{3\delta} \right]^{1/2}. \quad (2.35)$$

Using (2.34) and (2.21) in (2.19), we easily write the matrix of the metric tensor as

$$g_{ij} = \int \phi_i(x) \phi_j(x) dx = \|\phi\|^2 \delta_{ij}. \quad (2.36)$$

Adapting (2.16) to the finite-dimensional setting

$$\sum_{ij} g_{ij} \partial_t \zeta_j d\zeta_i = \sum_i \frac{\partial \mathcal{E}(\zeta)}{\partial \zeta_i} d\zeta_i \quad (2.37)$$

and using (2.36) we immediately obtain the Ginzburg-Landau equation in the  $\zeta$ -coordinates

$$\partial_t \zeta_i = -\frac{1}{\|\phi_i\|^2} \frac{\partial \mathcal{E}(\zeta)}{\partial \zeta_i}. \quad (2.38)$$

Constrained Allen-Cahn equation. In order to understand how the presence of the conserved quantity affects the asymptotic behavior of a gradient system and to prepare ourselves for the study of the Cahn-Hilliard equation, let us consider an artificial example: the constrained Allen-Cahn equation. The flow for this system is obtained by taking the regular Allen-Cahn gradient flow under the constraint that the total integral of the field  $u(x)$  be preserved. The equation reads

$$\partial_t u = \delta \partial_{xx}^2 u - \frac{1}{\delta} V'(u) + \mu, \quad \mu = \frac{1}{\delta L} \int_0^L V'(u) dx, \quad (2.39)$$

where  $\mu$  is the Lagrange multiplier for the constraint. The leading order evolution on the  $\tau = t/\delta$  time scale is a parametrically-coupled ‘system’ of ODEs (analogue of (2.4))

$$\partial_\tau u = -V'(u) + \frac{1}{L} \int_0^L V'(u) dx, \quad (2.40)$$

whose solution again converges as  $\tau \rightarrow \infty$  to piecewise constant functions assuming the values  $\pm 1$  almost everywhere<sup>12</sup> with the same boundary layers as in the regular Ginzburg-Landau equation.

Since the dynamics is constrained, we will take a projection of the vectors on the tangent space as described in the end of Section 2.3 in order to exclude the directions violating the constraint. In the  $\zeta$ -coordinates, the total integral of the field is defined by

$$\hat{\mathcal{F}} = 2 \sum_i (-1)^i \zeta_i + L, \quad (2.41)$$

and therefore the constraint simply restricts the motion to the kernel of the gradient of  $\hat{\mathcal{F}}$

$$d\hat{\mathcal{F}} = 2 \sum_i (-1)^i d\zeta_i, \quad \ker d\hat{\mathcal{F}} = \text{span} \left\{ \sum_j \hat{P}_{ij} \partial_{\zeta_j} \right\} \quad (2.42)$$

---

<sup>12</sup>The condition that  $\mathcal{E} = \mathcal{O}(\delta)$  should also be employed of course.

where  $\hat{P}_{ij}$  is the matrix of the projection operator  $\hat{\mathbf{P}} = \sum_{ij} \hat{P}_{ij} \boldsymbol{\partial}_{\zeta_i} \otimes \mathbf{d}\zeta_j$ ,

$$\hat{P}_{ij} = \delta_{ij} - \frac{1}{N}(-1)^{i+j}, \quad (2.43)$$

and  $N$  is the number of kinks (which equals to the dimension of the slow manifold). Notice that  $\text{span}\{\boldsymbol{\partial}_{\lambda_i}\}$  has dimension  $N - 1$ . Now the constrained Ginzburg-Landau gradient flow can be written as

$$\hat{\mathbf{P}} \hat{\mathbf{g}} \hat{\mathbf{P}} \partial_t = \mathbf{d}\mathcal{E}(\boldsymbol{\zeta}) \hat{\mathbf{P}}, \quad (2.44)$$

where  $\hat{\mathbf{g}}$  has the same matrix (2.36) as the one for the regular Ginzburg-Landau equation. Componentwise, the last equation reads

$$\partial_t \zeta_i = -\frac{1}{\|\phi_i\|^2} \sum_j \hat{P}_{ij} \frac{\partial \mathcal{E}(\boldsymbol{\zeta})}{\partial \zeta_j}, \quad (2.45)$$

where we also used the fact that we can freely invert the matrix  $\hat{P}$  on the kernel of  $\mathbf{d}\hat{\mathcal{F}}$  (it is just the identity matrix there).

**Cahn-Hilliard equation.** The Cahn-Hilliard equation (1.2) in one dimension reads

$$\partial_t u = -\partial_{xx}^2 (\delta \partial_{xx}^2 u - \frac{1}{\delta} V'(u)), \quad V(u) = \frac{1}{4}(1 - u^2)^2. \quad (2.46)$$

To identify the slow manifold let us first undertake an asymptotic analysis similar to what we did for the Ginzburg-Landau equation. Expanding

$$u(x, t) = v^{(0)}(x, \tau) + \delta^2 v^{(1)}(x, \tau) + \mathcal{O}(\delta^4), \quad \tau = t/\delta, \quad (2.47)$$

we obtain

$$\partial_\tau v^{(0)} = \partial_{xx}^2 V'(v^{(0)}). \quad (2.48)$$

Notice, that the equation for  $v^{(0)}$  is not an ODE as (2.4), however, the dynamics is still attractive to the states  $V'(v^{(0)}) = \text{const}$  as  $\tau \rightarrow \infty$ . Together with the condition that energy be finite, this necessarily requires convergence to  $v^{(0)} = \pm 1$ , in which case  $V'(\pm 1) = 0$ . As before, expansion near the layers where  $v^{(0)}$  jumps from  $-1$  to  $+1$  should be modified to account for the  $y = x/\delta$  scale, which immediately yields that the boundary layer has the same form  $\tanh(\pm y/\sqrt{2})$  as the kink for the Allen-Cahn equation.

Let us now derive equations for the motion on the slow manifold in the  $\boldsymbol{\zeta}$ -coordinates. The conserved quantity  $\hat{\mathcal{F}}$  defining the degenerate direction is the total integral of the field  $u(x)$  and, together with its gradient, is defined in (2.41) and (2.42). Rewriting expression (2.19) in the  $\boldsymbol{\zeta}$ -parametrization we can formally write the matrix of the metric tensor restricted to the slow

manifold as

$$g_{ij} = \int \partial_x^{-1} \phi_i(x) \partial_x^{-1} \phi_j(x) dx. \quad (2.49)$$

However, as was mentioned before, this expression is not uniquely defined, which is related to degeneracy of the  $\partial_x$  operator. Restricting the dynamics to the kernel of  $\mathbf{d}\hat{\mathcal{F}}$  by means of the projection operator introduced in (2.43) we obtain the expressions for the matrix of the ‘corrected’ metric tensor  $\hat{\mathbf{P}} \hat{\mathbf{g}} \hat{\mathbf{P}}$

$$\tilde{g}_{ij} = \int \partial_x^{-1} \sum_{i'} \hat{P}_{ii'} \phi_{i'}(x) \partial_x^{-1} \sum_{j'} \hat{P}_{jj'} \phi_{j'}(x) dx, \quad (2.50)$$

where  $\partial_x^{-1}$  is now defined to produce functions with the total integral 0. One can calculate this matrix straightforwardly, obtaining evolution equations in terms of kink locations  $\zeta_i$ . However it is more convenient to do it in a different way. Instead of using the  $\zeta$ -coordinates, let us parametrize the slow manifold by  $\xi_i$  given implicitly by

$$\zeta_i = \frac{1}{2}(\xi_i + \xi_{i+1}), \quad (2.51)$$

The transformation formulae analogous to (2.34) read

$$\mathbf{d}u_{\boldsymbol{\xi}}(x) = \sum_i \psi_i(x) \mathbf{d}\xi_i, \quad \psi_i(x) = \frac{1}{2}[\phi_i(x) + \phi_{i-1}(x)]. \quad (2.52)$$

The matrix of the metric tensor is calculated easily in the basis  $\{\boldsymbol{\theta}_{\xi_i} \otimes \mathbf{d}\xi_j\}$  since  $\partial_x^{-1}$  is well-defined on functions  $\psi_i(x)$  which have the total integral 0:

$$\partial_x^{-1} \psi_i(x) = (-1)^i \left[ \theta(x - \zeta_{i-1}) \theta(\zeta_i - x) + \frac{1}{L} (\zeta_{i-1} - \zeta_i) \right] + \mathcal{O}(\delta), \quad (2.53)$$

where  $\theta(x)$  is a step-function. Introducing  $\lambda_i = \zeta_i - \zeta_{i-1} = 1/2(\xi_{i+1} - \xi_{i-1})$  and employing formula (2.19) we find

$$\tilde{g}_{ii} = \frac{\lambda_i}{L}(L - \lambda_i), \quad \tilde{g}_{ij} = -\frac{(-1)^{i+j}}{L} \lambda_i \lambda_j \quad i \neq j. \quad (2.54)$$

Equation for the Cahn-Hilliard flow can now be written as

$$\sum_j \tilde{g}_{ij} \partial_t \xi_j = -\frac{\partial \mathcal{E}(\boldsymbol{\xi})}{\partial \xi_i}. \quad (2.55)$$

### 2.4.3 Deterministic coarsening via collapse of the smallest domain

Deterministic dynamics on the slow manifold is in fact frozen, i. e., on all time scales of order  $\mathcal{O}(\delta^n)$  multi-kink solutions are stationary<sup>13</sup>. Motion can only be observed on an exponentially long time scale, and is effectively stimulated by weak attraction among the kinks. This interaction is the result of an exponentially small mismatch, which appears when one constructs the composite multi-kink solution connecting single kinks, which are only exact solutions on the entire line  $\mathbb{R}$ .

In order to understand the nature of this interaction, let us consider a two-kink solution on the line

$$u(x, t) = \tanh \left[ \frac{\zeta - x}{\sqrt{2}\delta} \right] + \tanh \left[ \frac{\zeta + x}{\sqrt{2}\delta} \right] - 1 + \mathcal{O} \left( \exp \{ -\sqrt{2}\zeta/\delta \} \right). \quad (2.56)$$

This is a configuration, symmetric about 0, of two kinks separated by  $2\zeta$ . We can estimate the energy of this configuration by substituting this ansatz into (1.4) and collecting the principal terms<sup>14</sup>

$$\mathcal{E}[u] = \mathcal{O} \left( -\exp \{ -\sqrt{2}\zeta/\delta \} \right). \quad (2.57)$$

This implies an exponentially weak attraction between successive kinks. In a similar manner, we can consider the general multi-kink solution by formally writing an expression for the energy in the form

$$\mathcal{E}(\zeta) \sim \sum_i \exp \left\{ \frac{1}{\sqrt{2}\delta} (\zeta_i - \zeta_{i+1}) \right\}. \quad (2.58)$$

This expression, in fact, can be rather misleading. The reason is that only the contribution of the two nearest kinks is essential, whereas all other interactions are exponentially weak compared to this one. When considering the dynamics, one can assume that all the kinks but the nearest two do not move at all, while these two approach and annihilate each other. We then consider the next nearest pair as moving, and so on. This scenario of coarsening is called the successive domain elimination and was first proposed by A. J. Bray, B. Derrida and C. Godrèche [5].

In the case of the constrained Ginzburg-Landau and Cahn-Hilliard dynamics, this coarsening scenario is still valid, except that there also appears the induced movement of all the other kinks. Therefore by the time the two nearest kinks have mutually annihilated, the rest of them also shift slightly to compensate for the change in the total integral of the field. This shift is the same for all kinks in the constrained Ginzburg-Landau equation, however, for the Cahn-Hilliard equation it diminishes with the distance from the two kinks which actively interact.

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<sup>13</sup>This can be seen if one substitutes a multi-kink ansatz into equations of motion, and observes that only an exponentially small inconsistency appears.

<sup>14</sup>We subtracted the constant value equal to the energy of the two kinks. The minus sign indicates that the remainder is negative.

## CHAPTER 3

### Stochastically perturbed systems

#### 3.1 General comments

Stochastically perturbed problems of the form (1.3) have attracted significant attention in the past few decades. Let us mention the most relevant references to our particular case. G. S. Katzenberger [24] considered diffusive dynamics of a system forced onto a slow manifold in the finite dimensional case. T. Funaki studied the motion of a single interface induced by the random forcing in the one-dimensional Ginzburg-Landau equation [21] and also, in the two dimensional Ginzburg-Landau equation, a modification of the motion by mean curvature induced by noise that is homogeneous in space [22]. T. Shardlow considered a stochastic perturbation of the one-dimensional Allen-Cahn equation in [35].

We consider the small noise limit  $\epsilon \ll \delta$  such that the structure of the slow manifold is not violated. The stochastically perturbed dynamics of (1.1) becomes

$$\partial_t u = \delta \Delta u - \frac{1}{\delta} V'(u) + \sqrt{\epsilon} \xi(\mathbf{x}, t), \quad (3.1)$$

where  $\xi(\mathbf{x}, t)$  is a Gaussian stochastic process which we will assume to be  $\delta$ -correlated in time. The question of spatial correlations is more complicated and requires additional consideration. It turns out that in the one-dimensional situation it is possible to have  $\delta$ -correlated noise, but in higher dimensions equation (3.1) can only be properly defined if the noise has finite correlation length.

An additional comment should be made concerning the scaling of  $\epsilon$  and  $\delta$ . As was mentioned, the condition  $\epsilon \ll \delta$  is a simple requirement that the structure of the slow manifold remains the same as in the deterministic case. This alone however is not enough since one can expect certain large deviations to appear even as  $\epsilon \rightarrow 0$ . Although their probability diminishes exponentially fast, they still may appear if the length and time scales of the domain in which we consider our equation are large enough<sup>15</sup>. In fact, this phenomenon is well known and is called nucleation. We will discuss it briefly in Section 3.3 and Appendix A.

**Geometric approach.** Similarly to deterministic systems, we can cast the stochastically perturbed ones into the same covariant form (2.16)

$$\hat{\mathbf{g}} \partial_t = -\mathbf{d}\mathcal{E} + \sqrt{\epsilon} \boldsymbol{\xi}, \quad \boldsymbol{\xi} = \int \mathbf{d}\mathbf{x} \xi(\mathbf{x}) \mathbf{d}u(\mathbf{x}). \quad (3.2)$$

Here  $\boldsymbol{\xi}$  is a 1-form which appears as a consequence of the stochastic perturbation. We will call it the stochastic form. The restriction to the slow manifold is applied in exactly the same way as

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<sup>15</sup>Of course, this only occurs if we rescale the time and space with  $\epsilon$  and  $\delta$ , which is the case when we study the one-dimensional problem where this scaling is necessary to obtain the system admissible for statistical study.

(2.18), yielding the transformation of the components of  $\boldsymbol{\xi}$ ,

$$\boldsymbol{\xi}_\ell = \int d\mathbf{x} \xi_\ell(\mathbf{x}) d\ell(\mathbf{x}), \quad \xi_\ell(\mathbf{x}) = \int \xi(\mathbf{y}) D_{\ell(\mathbf{x})} u(\mathbf{y}) d\mathbf{y}. \quad (3.3)$$

Its covariance matrix provides a complete characterization of the noise on the slow manifold and is given by

$$\langle \xi_\ell(\mathbf{x}) \xi_\ell(\mathbf{y}) \rangle = \int d\mathbf{x}' \int \langle \xi(\mathbf{x}') \xi(\mathbf{y}') \rangle D_{\ell(\mathbf{x}')} u(\mathbf{x}') D_{\ell(\mathbf{y}')} u(\mathbf{y}') d\mathbf{y}'. \quad (3.4)$$

## 3.2 Examples

All the machinery of the dynamics reduction works in exactly the same way as in the deterministic setting. The effect of the stochastic forcing only appears as a perturbation of the energy gradient. Therefore, it is sufficient to calculate the covariance of the noise in the coordinates of the slow manifold to obtain the complete description of the reduced dynamics.

In one dimension, we will reduce the stochastic Ginzburg-Landau equation to a diffusion-annihilation process, which will be the subject of the study in Chapter 4 in the context of the coarsening phenomenon.

### 3.2.1 Stochastic Ginzburg-Landau equation in several dimensions

While deriving the equations (on the slow manifold) for  $\ell$  in the deterministic case, we obtained the evolution equations for all of its level sets. There was, however, much redundant information since we are only interested in the 0-level set which defines the interface. In order to simplify the calculations for the influence of the stochastic forcing, let us only consider the 0-level set and obtain the covariance matrix on it. Using (3.4) and (2.25), we find that for  $\ell(\mathbf{x}) = \ell(\mathbf{y}) = 0$

$$\langle \xi_\ell(\mathbf{x}) \xi_\ell(\mathbf{y}) \rangle = \frac{\langle \xi(\mathbf{x}) \xi(\mathbf{y}) \rangle}{2\delta^2 |\nabla \ell(\mathbf{x})| |\nabla \ell(\mathbf{y})|}. \quad (3.5)$$

Because we only obtained the covariance matrix on the 0-level set of  $\ell$ , we cannot use it to make a stochastic modification of (2.32), which describes the global evolution of  $\ell$ . Instead, we modify (2.33) to find an equation for the normal velocity  $v(\mathbf{x})$  of the 0-level set alone:

$$v(\mathbf{x}) = \delta \kappa_\ell(\mathbf{x}) + \frac{3\sqrt{\epsilon}}{4} \xi(\mathbf{x}). \quad (3.6)$$

We can see that even in the asymptotic limit  $\epsilon = \mathcal{O}(\delta)$  and  $\delta \rightarrow 0$  stochastic term may interact non-trivially with the dynamics.



### 3.2.2 Examples in one dimension

Ginzburg-Landau equation. In one dimension, the stochastic Ginzburg-Landau equation reads

$$\partial_t u = \delta \partial_{xx}^2 u - \frac{1}{\delta} V'(u) + \sqrt{\epsilon} \xi(x, t), \quad (3.7)$$

where  $\xi(x, t)$  is now a regular space-time white noise process with the covariance matrix  $\langle \xi(x_1, t_1) \xi(x_2, t_2) \rangle = \delta(x_1 - x_2) \delta(t_1 - t_2)$ . In the limit as  $\delta \rightarrow 0$ , deterministic motion is still constrained on the slow manifold if  $\epsilon \ll \delta$ .

Using the same parametrization as in the deterministic setting, we get the same metric tensor, and the components of the stochastic form read

$$\xi_i = \int \phi_i(x) \xi(x) dx. \quad (3.8)$$

Therefore, the equation for  $\zeta_i$  on the slow manifold reads

$$\partial_t \zeta_i = -\frac{1}{\|\phi_i\|^2} \left[ \frac{\partial \mathcal{E}(\zeta)}{\partial \zeta_i} - \sqrt{\epsilon} \xi_i(t) \right]. \quad (3.9)$$

By calculating the covariance matrix of  $\boldsymbol{\xi}$ , we see that the noises controlling each individual kink are independent

$$\langle \xi_i(t_1) \xi_j(t_2) \rangle = \int dx \int dy \phi_i(x) \phi_j(y) \langle \xi(x) \xi(y) \rangle dy = \|\phi_i\|^2 \delta_{ij} \delta(t_1 - t_2) \quad (3.10)$$

The first gradient term, which is induced by the deterministic dynamics (2.38), is exponentially weak in  $\delta$ , and therefore by scaling  $\epsilon$  as some power of  $\delta$  we can ensure that it does not affect the dynamics (up to the very moment of the kink collision). Therefore in such a scaling, we end up with the purely diffusive kink motion

$$\partial_t \zeta_i = \frac{\sqrt{\epsilon}}{\|\phi_i\|} \beta_i(t), \quad (3.11)$$

where  $\beta_i(t)$  are now independent standard white noises. In particular, for the Ginzburg-Landau potential we find

$$\partial_t \zeta_i = \sqrt{\mathcal{D}/2} \beta_i(t), \quad \mathcal{D} = \frac{3\sqrt{2}}{8} \epsilon \delta. \quad (3.12)$$

Thus a kink can be associated with a particle undergoing Brownian motion with the diffusion coefficient  $\mathcal{D}$ . The dynamics of the whole system is therefore equivalent to a diffusion-annihilation process.

At the point of kink collision, depending on the potential  $V(u)$ , different phenomena may arise. If the collision between a kink and the corresponding antikink occurs, then the two annihilate each other. The deterministic contribution in this case only accelerates the annihilation on the  $\mathcal{O}(1/\delta)$  time-scale. If the two kinks have different colors (as in a multi-well potential), annihilation

is not possible, and instead, the kinks serve as reflecting boundaries for one another.

**Constrained Ginzburg-Landau.** Let us write down the equation for the stochastic constrained Ginzburg-Landau dynamics

$$\partial_t u = \delta \partial_{xx}^2 u - \frac{1}{\delta} V'(u) + \sqrt{\epsilon} \xi(x, t) + \mu, \quad \mu = \frac{1}{L} \int_0^L \left[ \frac{1}{\delta} V'(u) - \sqrt{\epsilon} \xi \right] dx \quad (3.13)$$

Similarly to (2.44), we obtain the equation for the stochastic vector field

$$\hat{\mathbf{P}} \hat{\mathbf{g}} \hat{\mathbf{P}} \partial_t = (\mathbf{d}\mathcal{E}(\zeta) + \sqrt{\epsilon} \boldsymbol{\xi}) \hat{\mathbf{P}}, \quad (3.14)$$

where  $\hat{\mathbf{P}}$  is again the projection operator defined in (2.43). Componentwise, the last equation reads

$$\partial_t \zeta_i = -\frac{1}{\|\phi_i\|^2} \sum_j \hat{P}_{ij} \left[ \frac{\partial \mathcal{E}(\zeta)}{\partial \zeta_j} - \sqrt{\epsilon} \xi_j(t) \right]. \quad (3.15)$$

Neglecting the deterministic dynamics in the asymptotic limit, we obtain the following set of equations

$$\partial_t \zeta_i = \frac{\sqrt{\epsilon}}{\|\phi_i\|^2} \sum_j \hat{P}_{ij} \|\phi_j\| \beta_j(t). \quad (3.16)$$

In particular for the Ginzburg-Landau potential

$$\dot{\zeta}_i = \left[ \frac{3\sqrt{2}}{4} \epsilon \delta \right]^{1/2} \sum_{j=1}^N \hat{P}_{ij} \beta_j(t). \quad (3.17)$$

### 3.3 Scalings for coarsening and nucleation

The following part of this work is dedicated to studies of the coarsening phenomenon in the one dimensional stochastic Ginzburg-Landau equation. We have so far considered this system on the finite interval  $x \in (0, L)$ . In this case, the system will eventually coarsen completely and all the kinks will annihilate. One can, however, rescale the space to obtain asymptotic dynamics on the entire line. Certainly, because of the diffusive motion, the time interval  $T$ , during which we observe our system, should be rescaled respectively as<sup>16</sup>  $T = L^2/\mathcal{D}$ . This restriction appears in order to be consistent with the small noise asymptotics, i. e., to remain in the regime in which the large deviations from the slow manifold are not allowed. Since the probability of large deviations scales as  $\Delta^{-1} \exp\{-\mathcal{E}/\epsilon\}$ , where  $\Delta$  is the space-time scale of such a deviation and  $\mathcal{E}$  is the corresponding energy fluctuation, we need to require that  $LT = o(\Delta \exp\{\mathcal{E}/\epsilon\})$ . Obviously, scaling  $L$  and  $T$  polynomially in  $\epsilon$  will achieve this purpose.

The large deviations mentioned above lie at the core of the nucleation phenomenon. The essence of this process is the creation of a new domain (kink-antikink pair). Nucleation is respon-

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<sup>16</sup> $\mathcal{D}$  is the diffusion coefficient for the kinks defined in (3.12).

sible for the ability of the system to reach a **statistical equilibrium** state as time goes to infinity. In the scaling we have considered for the coarsening problem this never occurs and the system coarsens forever in a self-similar regime rather than reaching a steady state. We refer the reader to the Appendix A for additional information concerning nucleation.

**Equilibrium states.** The nucleation rate is exponentially small in  $\epsilon$  and therefore, in order to be able to observe nucleations, we need to consider space-time regions with area exponentially large in  $\epsilon$ . There exist two distinct limits with totally different equilibrium states.

- **Finite space — long time.** The coarsening in such system terminates very fast and the entire field switches to one of the  $u = \pm 1$  states. Once in a while, a successful nucleation occurs, which flips the whole field to a different meta-stable state, and so on. This process has been studied by W. E. W. Ren, and E. Vanden-Eijnden [14]
- **Long space — long time.** A different situation occurs when both space and time are scaled exponentially (time is always scaled as space squared to be able to observe diffusion). Here, coarsening and nucleation interplay non-trivially, and one observes persistent evolution of domains, their annihilation due to coarsening, and creation of new ones in the process of nucleation.

## CHAPTER 4

### Brownian particles and related systems

This chapter is devoted to a statistical analysis of one-dimensional lattice spin and particle systems with voters dynamics and their continuous limits. We build a complete statistical description of such systems that rests on different correlation functions and hierarchies of equations for their temporal evolution. The foundations of the theory for an infinite number of coalescing random walkers and continuous scaling limits of such system has been studied by R. Arratia [2].

#### 4.1 Spin lattices and their statistical description

We define a one-dimensional spin lattice to be a function  $\eta : \mathbb{Z} \rightarrow \Omega$  mapping integer numbers onto a set  $\Omega$  of values, which any particular site (spin) can assume. Throughout this discussion,  $\Omega = \{1, \dots, q\}$  ( $q$  may sometimes go to infinity), which corresponds to the  $q$ -state lattice model, and  $\eta_i$  is the value of the spin with coordinate  $i$ . In correspondence to every spin system, we introduce a dual system of particles which are associated with the transition layers from one spin value to another, i. e., in every case  $\eta_i \neq \eta_{i+1}$ , we put a particle at the location  $i$  which now separates domains of spins with the same value. To make a correspondence between the spin and particle systems we also need to assign each particle a color which equals  $\eta_i$ .

There are several ways to arrive at a probabilistic description of such a spin system. The basic way is based on the family of spin correlation functions

$$\varphi^{(k)}(z_1, \dots, z_k | \omega_1, \dots, \omega_k) \tag{4.1}$$

— the probabilities that  $\eta_{z_i} = \omega_i$ . The corresponding particle correlation functions

$$\varpi^{(k)}(z_1, \dots, z_k | \omega_1, \dots, \omega_k) \tag{4.2}$$

are the probabilities to have particles with colors  $\omega_i$  located at positions  $z_i$ . For notational convenience we will further on use vector notation ( $\mathbf{z}$  and  $\mathbf{\omega}$ ), assuming that the number of components in the corresponding vector equals the order  $k$  of the correlation function. We will also always assume that  $(\forall i < j) z_i < z_j$  and consider  $\varphi^{(k)}$  and  $\varpi^{(k)}$  in the domains  $z_1 < \dots < z_k$ , setting them to 0 on the boundary. Another way to describe the spin lattice is based on the inter-particle probability densities  $\varrho^{(k)}$  which are obtained from  $\varpi^{(k)}$  with the additional condition that there are no particles between each two specified locations.

We call the lattice homogeneous if the spin and particle correlation functions depend only on the difference of  $z_i$  rather on the coordinates themselves. In this case for every particular realization

of the lattice, one can obtain the correlation functions via spatial averaging, for example

$$\varphi^{(k)}(z_1, \dots, z_k | \omega_1, \dots, \omega_k) = \lim_{N \rightarrow \infty} \frac{1}{2N+1} \sum_{i=-N}^N \prod_{j=1}^k \delta_{\eta_{i+z_k}, \omega_k}. \quad (4.3)$$

The family of inter-particle densities is especially convenient because the  $\varrho^{(k)}$  form a consistent hierarchy, i. e., the lower-order densities can be obtained by summation over the ‘extra’ variables of the higher-order densities

$$\varrho^{(k)}(z_1, \dots, z_k | \omega_1, \dots, \omega_k) = \sum_{\omega \in \Omega} \sum_{z=z_k+1}^{\infty} \varrho^{(k+1)}(z_1, \dots, z_k, z | \omega_1, \dots, \omega_k, \omega). \quad (4.4)$$

## 4.2 Voters model

Let us now describe the dynamics of our spin system. Suppose that every spin has an independent Poisson clock which ticks with rate  $2D$ , i. e., the probability for the clock to tick in an infinitesimal time interval  $dt$  is equal to  $2D dt$ . When this happens, the spin chooses either its right or left neighbor (with probability  $1/2$ ) and takes its value (vote). Such an evolution is called voters dynamics and the system of spins with  $q$  states is called the  $q$ -states Potts model.

There is, of course, a corresponding random walk of the particles in the dual system. Indeed, whenever the clock ticks for the spin whose neighbors have the same value, effectively nothing changes, so the only evolution one can observe happens on the boundaries of the domains of spins with the same value. This is exactly a random walk of the corresponding particles. Moreover, when two kinks collide and some domain completely disappears, particles can either annihilate or coalesce, depending on the value of spins on the right and on the left of the vanishing domain.

Let us emphasize the two special cases in which the number of values a spin can take is  $q = 2$  and  $q = \infty$ . The voters dynamics associated with the former is called diffusion-annihilation and corresponds to the regular Ising model. In the latter case it is called diffusion-coalescence. These terms come from the fact, that provided we begin from an initial condition with random  $\eta_i$ , particles always disappear upon collision in case  $q = 2$ , whereas when  $q = \infty$  they coalesce (no two spins have the same value at  $t = 0$ ). Let us notice that voters dynamics in the lattice system is independent of  $q$ , so the difference between Potts models with different  $q$  is completely contained in the initial condition. In particular, the coalescing ( $q = \infty$ ) model contains in itself all other models. Indeed, let  $\theta_0(i)$  be the initial condition for some configuration. We can instead evolve the system with  $\eta_i^0 = i$  and afterwards assign new values to the spins as  $\eta_i = \theta_0(\eta_i)$ .

### 4.2.1 Backward random walks

A very important observation is that there is a random walk **backwards** in time associated with voters dynamics, namely for every spin it is the history of its value. Moreover, one can notice that these backward random walks are always coalescing. Indeed if at some point the histories of

two different spins can be traced to the same ‘ancestor,’ they obviously ‘coalesce’ and further-on traverse the same trajectory<sup>17</sup>. As a consequence, we can determine the value of any spin at any time  $t$  by tracing backwards its value to the initial state. For the coalescence problem, by using this reasoning, we can tell whether some particular spins have the same value — it is just a probability that the backward random walks starting at their respective coordinates have coalesced.

Let us for a while concentrate on the diffusion-coalescence problem to establish a connection between inter-particle probability densities and **collisional patterns** of coalescing random walks. First of all, we notice that if two spins have the same value, all the spins in-between also have the same value, so the probability that in a set of successive spins all of them belong to the same domain is nothing more than the probability that the backward random walks starting on the boundaries of the domain have coalesced. A particle in the dual system appears when two adjoining spins have different values, which means that the backward random walks have not coalesced. Let us introduce

$$\mathcal{C}_t^{(k)}[z_1 \cdot z_2 \cdot z_3 \cdot \dots \cdot z_k], \quad (4.5)$$

— the probabilities of different collisional patterns. The expression in the square brackets is a symbolic representation of a particular pattern in the following manner. The particles begin at locations  $z_i$  at time 0 and move until time  $t$ . We put the ‘|’ separator instead of ‘.’ in the case when none of the particles to the left of it collided with the particles to the right of it. We put ‘the separator ;’ instead of ‘.’ if we do not care whether the particles it separates collided or not, and we remove ‘.’ altogether if respective particles have collided. For example  $\mathcal{C}_t^{(k)}[z_1|z_2;z_3|z_4z_5]$  is the probability that the first particle has not collided with any of other particles, fourth and fifth have collided with each other, but did not collide with the second and the third. Of course this notation is not enough to embrace all possible collisional patterns, but nevertheless it is sufficient for the purposes of this work.

Now it is easy to see how one can express  $\varrho^{(k)}$  and  $\varpi^{(k)}$  through the probabilities of collisional patterns (we disregard colors since for the  $q = \infty$  model all the colors may be assigned at random at any time)

$$\begin{aligned} \varrho^{(k)}(z_1, \dots, z_k) &= \mathcal{C}_t^{(2k)}[z_1|z_1 + 1 \ z_2|z_2 + 1 \ z_3|z_3 + 1 \ \dots \ z_k|z_k + 1] \\ \varpi^{(k)}(z_1, \dots, z_k) &= \mathcal{C}_t^{(2k)}[z_1|z_1 + 1; z_2|z_2 + 1; z_3|z_3 + 1; \dots; z_k|z_k + 1]. \end{aligned} \quad (4.6)$$

Appendix B covers extensively this topic for continuous Brownian motions.

### 4.3 Evolution equations

Since we are interested in the statistical description of spin lattices, we should derive evolution equations for the correlation functions generated by the voters dynamics. The easiest way

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<sup>17</sup>Backwards in time, of course.

is to consider the family  $\varrho^{(k)}$  of inter-particle probability densities. As an example, we will derive such equations for the annihilating and coalescing case, disregarding the colors of the domains, i. e., we will only be interested in the distribution of domain lengths regardless of their colors. Generalizations are straightforward and can be easily derived as well.

**Coalescence.** In this case, all the colors are different for different domains and evolution equations easily follow by considering how some particular configuration can appear or disappear under the voters dynamics,

$$\begin{aligned} \partial_t \varrho^{(k)}(\mathbf{z}) &= D \left[ \Delta^{(k)} \varrho^{(k)} + \sum_{i=2}^{k-1} (\varrho^{(k+1)}(\dots z_i - 1, z_i \dots) + \varrho^{(k+1)}(\dots z_i, z_i + 1 \dots)) \right] \\ \partial_t \varrho^{(1)}(z) &= D \left[ \Delta^{(1)} \varrho^{(1)}(z) - \varrho^{(2)}(z - 1, z) - \varrho^{(2)}(z, z + 1) \right]. \end{aligned} \quad (4.7)$$

Here  $\Delta^{(k)}$  is the discrete Laplacian

$$\Delta^{(k)} \varrho^{(k)}(z_1, \dots, z_k) = \varrho^{(k)}(z_1 - 1 \dots) - 2\varrho^{(k)}(z_1 \dots) + \varrho^{(k)}(z_1 + 1 \dots) + \dots \quad (4.8)$$

The discrete Laplacian in (4.7) appears as a direct consequence of the diffusive dynamics of the particles, whereas the other terms correspond to the creation of some particular state in the process of coalescence, e. g., every term in the sum in (4.7) corresponds to the probability of coalescence of the particle located at  $z_i$  with the one to the left or to the right it.

**Annihilation.**

$$\begin{aligned} \partial_t \varrho^{(k)}(\mathbf{z}) &= D \left[ \Delta^{(k)} \varrho^{(k)} + 2 \sum_{i=1}^{k-1} \hat{C}_i^{(k)} \varrho^{(k+2)} - \varrho^{(k+1)}(z_1 - 1, z_1 \dots) \right. \\ &\quad \left. - \varrho^{(k+1)}(z_1, z_1 + 1 \dots) - \varrho^{(k+1)}(\dots z_k - 1, z_k) - \varrho^{(k+1)}(\dots z_k, z_k + 1) \right], \end{aligned} \quad (4.9)$$

where the collision operator is

$$\hat{C}_i^{(k)} \varrho^{(k+2)} = \sum_{z=z_i+1}^{z_{i+1}-2} \varrho^{(k+2)}(\dots z_i, z, z + 1, z_{i+1} \dots). \quad (4.10)$$

The collisional part corresponds to the creation of a certain state by the annihilation of a pair of particles and creation of a domain in the process. The other terms correspond to the destruction of a given state by the collision with a particle from the outside.

In both cases, the consistency condition (4.4) for the hierarchies can be easily verified by direct summation, albeit there is no summation over the spin values, since we disregarded them at the beginning.

### 4.3.1 Continuous limits

In order to obtain the appropriate continuous limits of the equations discussed in the previous section we send the lattice spacing  $dx$  to 0 and introduce new coordinates  $x_i = i dx$ , diffusion coefficient  $\mathcal{D} = D dx^{-2}$  and probability densities

$$\rho^{(k)}(x_1 \dots, x_k) = \varrho^{(k)}(dx z_1, \dots, dx z_k) dx^{-k}. \quad (4.11)$$

The same scaling limit can be applied to obtain continuous equivalents of the inter-particle correlation functions  $\pi^{(k)}(x_1 \dots, x_k) = \varpi^{(k)}(dx z_1, \dots, dx z_k) dx^{-k}$ .

Coalescence. Equations (4.7) for diffusion-coalescence become

$$\begin{aligned} \partial_t \rho^{(k)} &= \mathcal{D} \left[ \Delta^{(k)} \rho^{(k)} + 2 \sum_{i=2}^{k-1} \hat{\mathcal{F}}_i^{(k)} \rho^{(k+1)} \right], \\ \partial_t \rho^{(1)}(x) &= \mathcal{D} \left[ \partial_{xx}^2 \rho^{(1)}(x) - 2 \hat{\mathcal{F}}_1^{(1)} \rho^{(2)} \right], \end{aligned} \quad (4.12)$$

where  $\Delta^{(k)}$  is now the regular  $k$ -dimensional Laplacian, and  $\hat{\mathcal{F}}_i^{(k)}$  is the flux operator

$$\hat{\mathcal{F}}_i^{(k)} \rho^{(k+1)} = \left. \frac{\partial}{\partial x} \rho^{(k+1)}(\dots x_i, x \dots) \right|_{x=x_i}. \quad (4.13)$$

Notice that (4.12) should be solved in the domain  $x_1 < \dots < x_k$  with absorbing boundary conditions. In particular, the equation for  $\rho^{(2)}$  (as for  $\rho^{(1)}$ ) decouples from the rest of the hierarchy and reads

$$\partial_t \rho^{(2)}(x, y) = \mathcal{D} (\partial_{xx}^2 + \partial_{yy}^2) \rho^{(2)}(x, y). \quad (4.14)$$

We will be only interested in the homogeneous system, i. e., all the quantities only depend on the difference of the arguments, e. g.,  $\rho^{(2)}(x, y) = \rho^{(2)}(y - x)$ . In this case,  $\rho^{(1)}$  does not depend on  $x$  and its evolution (4.14) does not have a diffusive part.

Annihilation. Let us now consider the appropriate continuous limits for the annihilation equations (4.9)

$$\partial_t \rho^{(k)} = \mathcal{D} \left[ \Delta^{(k)} \rho^{(k)} + 2 \left( \sum_{i=1}^{k-1} \hat{\mathcal{C}}_i^{(k)} \rho^{(k+2)} - \hat{\mathcal{F}}_1^{(k)} \rho^{(k+1)} - \hat{\mathcal{F}}_k^{(k)} \rho^{(k+1)} \right) \right], \quad (4.15)$$

where the flux operator is introduced in (4.13) and the continuous version of the collision operator is defined by

$$\hat{\mathcal{C}}_i^{(k)} \rho^{(k+2)} = \int_{x_i}^{x_i+1} \frac{\partial}{\partial x} \rho^{(k+1)}(\dots x_i, y, x, x_{i+1} \dots) \Big|_{x=y} dy. \quad (4.16)$$



### 4.3.2 Domain-length probability densities

To emphasize the fact that we are interested in domain-length distributions in spatially homogeneous systems where  $\rho^{(k)}$  only depend on the difference of the arguments, we can introduce domain-length probability densities  $n^{(k)}$  by the following relations:

$$n^{(k)}(l_1, \dots, l_k) = \left[ \int_x^\infty \rho^{(2)}(x, y) dy \right]^{-1} \rho^{(k+1)}(x, x + l_1, \dots, x + l_1 + \dots + l_k). \quad (4.17)$$

These are the probability densities that by choosing  $k$  successive intervals at random we get the corresponding domain lengths. Let us consider some particular realization of the particle configuration. Labelling the particle locations by  $x_i$  for  $i = 0, \pm 1, \dots$ , we see that  $n^{(k)}$  are weakly equivalent to the following

$$n^{(k)}(l_1, \dots, l_k) = \lim_{n \rightarrow \infty} \frac{1}{2n+1} \sum_{i=-n}^n \prod_{j=1}^k \delta(x_{i+j} - x_{i+j-1} - l_j), \quad (4.18)$$

which is a simple reformulation of relation (4.3).

Based on the evolution equations (4.12) and (4.15) for  $\rho^{(k)}$ , it is not hard to derive the corresponding equations for  $n^{(k)}$ .

Coalescence.

$$\partial_t n^{(k)} = 2\mathcal{D} \left[ \Delta_\ell^{(k)} n^{(k)} + \sum_{i=1}^{k-1} n^{(k+1)}(\dots l_i, \downarrow, l_{i+1} \dots) + n^{(1)}(\downarrow) n^{(k)} \right]. \quad (4.19)$$

Here the arrow sign ‘ $\downarrow$ ’ designates the derivative with respect to the corresponding argument taken at 0. The modified Laplacian becomes

$$\Delta_\ell^{(k)} = \partial_{l_1 l_1}^2 - \partial_{l_1 l_2}^2 + \partial_{l_2 l_2}^2 - \dots - \partial_{l_{k-1} l_k}^2 + \partial_{l_k l_k}^2. \quad (4.20)$$

The equation for  $n^{(1)}$  is again decoupled, and reads

$$\partial_t n^{(1)} = 2\mathcal{D} (\partial_{ll}^2 n^{(1)} + n^{(1)}(\downarrow) n^{(1)}). \quad (4.21)$$

It has a similarity solution

$$n^{(1)}(l, t) = 2\xi e^{-\xi^2}, \quad \xi = l/\sqrt{8Dt}. \quad (4.22)$$

### Annihilation.

$$\begin{aligned} \partial_t n^{(k)} = 2\mathcal{D} \left[ \Delta_\ell^{(k)} n^{(k)} + \sum_{i=1}^{k-1} \int_0^{l_i} n^{(k+2)}(\dots l_{i-1}, l, \downarrow, l_i - l, l_{i+1} \dots) dl \right. \\ \left. - n^{(k+1)}(\downarrow, l_1 \dots) - n^{(k+1)}(\dots l_k, \downarrow) + 2n^{(1)}(\downarrow) n^{(k)} \right]. \end{aligned} \quad (4.23)$$

### 4.4 Coalescence as a super-process

It was mentioned earlier that the process of diffusion-coalescence is in a certain sense a ‘super-process’, i. e., if we know all of its details, we can obtain the solution to any Potts model. Indeed, let us assume that the initial condition is such that all the colors are generated randomly. By propagating the coalescence model, we can afterwards reassign  $q$  colors to the intervals, merging the neighbors which have the same color to obtain the solution to the  $q$ -state Potts model. In particular  $n_q^{(1)}$  for the  $q$ -state Potts is expressed with the use of all  $n_\infty^{(k)}$  for the coalescing case by

$$\begin{aligned} n_q^{(1)}(l) = \left( \frac{q-1}{q} \right)^2 \left[ n_\infty^{(1)}(l) + \frac{2}{q} \int_0^l n_\infty^{(2)}(l_1, l-l_1) dl_1 \right. \\ \left. + \frac{3}{q^2} \int_0^l dl_1 \int_0^{l-l_1} n_\infty^{(3)}(l_1, l_2, l-l_1-l_2) dl_2 + \dots \right]. \end{aligned} \quad (4.24)$$

In particular the first term corresponds to the case that a given domain is just a single domain from the coalescence process, the second term comes from the possibility that it was obtained by merging two domains, and so on. This indicates, that although by knowing all the details of the diffusion-coalescence process we in principle can extract information concerning any  $q$ -state Potts model, it is in fact hardly attainable since even for describing  $n_q^{(1)}(l)$ , we need to know all  $n_\infty^{(1)}(l)$ .

### 4.5 Decoupling the hierarchies

One of the possible decouplings of the hierarchies (4.20, 4.23) of equations for domain-length distributions consists of application of the formulas (B.7) and (B.13). Indeed, the continuous analogue of equation (4.6) for the inter-particle densities reads

$$\rho^{(k)}(x_1, \dots, x_k) = \lim_{dx \rightarrow 0} \frac{1}{dx^k} \mathcal{C}_t^{(2k)}[x_1|x_1+dx \ x_2|x_2+dx \ \dots \ x_k|x_k+dx]. \quad (4.25)$$

Therefore, one can explicitly calculate  $\rho^{(k)}$  for the diffusion-coalescence process in self-similar regime. These calculations, however, are practically impossible to undertake. Moreover, as was mentioned in the previous section, the entire hierarchy of  $\rho^{(k)}$  for the coalescence process is needed in order to obtain anything for the finite- $q$ -state Potts model.

Consequently, we suggest a systematic way to build consistent approximations of any degree of precision based on assumptions of the absence of correlations of lengths of different intervals. Let us notice that different possible closures of the hierarchy of correlation functions  $\varphi^{(k)}$  are discussed

by J-C. Lin, C. Doering and D. ben-Avraham in [27]. We introduce the conditional probability densities  $p(l_1[l_2, \dots, l_k])$  that given that the successive nearest neighbors of some interval have lengths  $l_2, \dots, l_k$ , the length of the latter is  $l_1$ . These conditional probabilities are connected to the  $n^{(k)}$ , introduced earlier, by the obvious relation

$$n^{(k)}(l_1, \dots, l_k) = n^{(k-1)}(l_2, \dots, l_k) p(l_1[l_2, \dots, l_k]). \quad (4.26)$$

Keeping this in mind and making various assumptions on  $p$ -s, we can express the higher-order  $n^{(k)}$  through the lower-order ones.

**Independent intervals.** Making the assumption that  $p(l_1[l_2, \dots, l_k]) = n^{(1)}(l_1)$ , i. e., the conditional probability density does not in fact depend on any condition, we basically assume that there are no correlations whatsoever in the lengths of different intervals. This ansatz provides us with the decoupling of the form

$$n^{(k)}(l_1, \dots, l_k) = n^{(1)}(l_1) \cdots n^{(1)}(l_k). \quad (4.27)$$

Since, in the coalescing case the equation for  $n^{(1)}$  decouples from the rest of the hierarchy, this closure allows us to obtain approximate expressions for  $n^{(1)}$  (as well as for any  $n^{(k)}$ ) for any  $q$ -state Potts model using (4.24)

$$n_q^{(1)}(l) = \left(\frac{q-1}{q}\right)^2 \left[ n^{(1)}(l) + \frac{2}{q} n_\infty^{(1)} * n_\infty^{(1)}(l) + \frac{3}{q^2} n_\infty^{(1)} * n_\infty^{(1)} * n_\infty^{(1)}(l) + \cdots \right], \quad (4.28)$$

where ‘\*’ denotes the convolution  $f * g(x) = \int_0^x f(y)g(x-y) dy$ . By taking the Laplace transformation  $\hat{n}(s) = \int_0^\infty n^{(1)}(l) e^{-sl} dl$ , we easily obtain

$$\hat{n}_q(s) = \frac{(q-1)^2 \hat{n}_\infty(s)}{(q - \hat{n}_\infty(s))^2}. \quad (4.29)$$

By using (4.22), we can express the Laplace transform of the self-similar solutions by

$$\hat{n}_q(s) = \frac{(q-1)^2 (1 - \sqrt{\pi}/2 s e^{s^2/4} \operatorname{erf}(s/2))}{((q-1) + \sqrt{\pi}/2 s e^{s^2/4} \operatorname{erf}(s/2))^2}. \quad (4.30)$$

**Nearest neighbors or Markovian approximation.** Instead of assuming total independence of the domain lengths, we can allow for correlation between the nearest (successive) domain lengths, i. e., set  $p(l_1[l_2, \dots, l_k]) = p(l_1[l_2])$ . Taking into account (4.26), we see that  $p(l_1[l_2]) = n^{(2)}(l_1, l_2)/n^{(1)}(l_2)$ , which provides us with expressions for any  $n^{(k)}$  using only  $n^{(1)}$  and  $n^{(2)}$

$$n^{(k)}(l_1, \dots, l_k) = \frac{n^{(2)}(l_1, l_2) \cdots n^{(2)}(l_{k-1}, l_{k-2})}{n^{(1)}(l_2) \cdots n^{(1)}(l_{k-1})}. \quad (4.31)$$

Here, we present figures with numerical simulations comparing the domain-length proba-

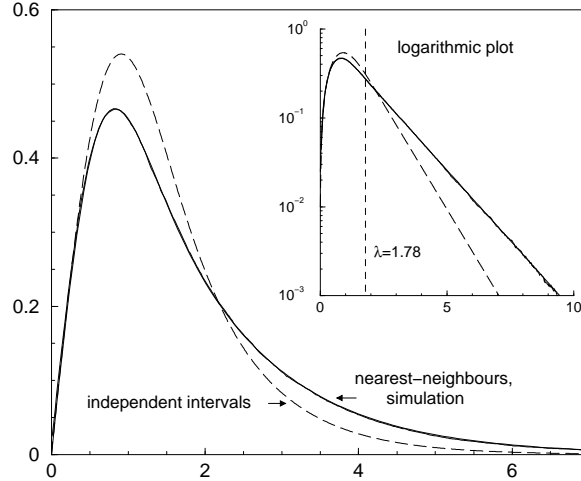


Figure 4.1: Scaling function of  $n^{(1)}$

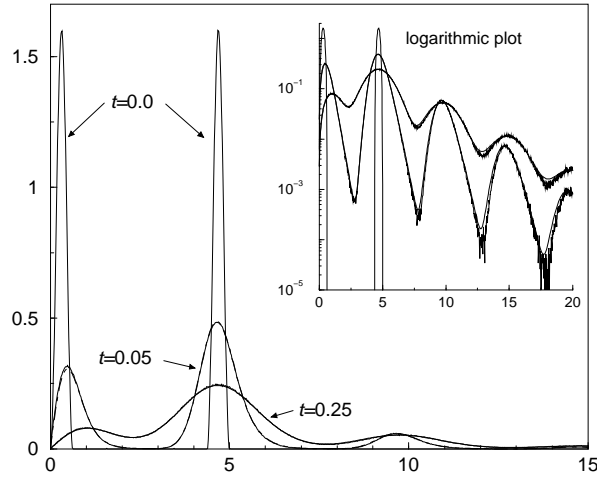


Figure 4.2: Relaxation of  $n^{(1)}(l, t)$

bility densities obtained by using the nearest-neighbor approximation with the approximation of independent intervals and direct simulations of an ensemble of particles on the ring. The direct simulations were performed with ensembles of  $10^6$  (initially) to  $10^4$  (at the end of the simulation) particles to ensure that the finiteness of the system does not affect the results. Initially, the intervals were generated independently with some probability density  $n_0^{(1)}(l)$ . Figure 4.1 displays the comparison of the scaling function (in the self-similar regime) of  $n^{(1)}$  obtained by using direct simulation, approximation of the independent intervals and Markovian approximation. Figure 4.2 displays the relaxation of  $n^{(1)}(l)$  from some initial distribution and comparison of the nearest-neighbor approximation and the direct simulation. As it is easy to see, the Markovian approximation is in excellent agreement with the direct simulations.

Higher-order closures. We can build an entire series of successive approximations by cutting the dependence on the neighbors at the  $j$ -th level, i. e., assuming that  $p(l_1[l_2, \dots, l_k]) = p(l_1[l_2, \dots, l_j])$ , ( $j < k$ ). As in the previous cases, this allows to express all higher-order densities as

$$n^{(k)}(l_1, \dots, l_k) = \frac{\prod_{i=1}^{k-j+1} n^{(j)}(l_i, \dots, l_{i+j-1})}{\prod_{i=2}^{k-j} n^{(j-1)}(l_i, \dots, l_{i+j-2})}. \quad (4.32)$$

We should also notice that different kinds of approximations appear depending on whether we apply these closures directly to the  $q$ -state Potts models or to the  $q = \infty$  coalescence process and then obtain the finite- $q$  model via relations similar to (4.24).

## APPENDIX A

### Tilted Ginzburg-Landau potential, nucleation and anomalous relaxation

By assuming that the minima of the potential  $V(u)$  are not equal, e. g., as in the tilted Ginzburg-Landau potential  $V(u) = \frac{1}{4}(1 - u^2)^2 + \gamma u$ , we obtain the system which may differ from those we considered before. The tilt  $\gamma u$  in the potential breaks the symmetry of the equilibrium states  $u = \pm 1$ , and only one of them remains stable under stochastic perturbations. It is especially easy to understand nucleation in this context.

The minima of the potential are slightly shifted (for small  $\gamma$ ), and are reached at  $u = u_{\pm} = \pm 1 + \gamma/2 + \mathcal{O}(\gamma^2)$ . The kink solutions of the deterministic system have the form  $\tanh[(ct \pm x)/\sqrt{2}\delta] + \gamma/2 + \mathcal{O}(\gamma^2)$  and are no more stationary, but propagate with constant velocity  $c = 3\gamma/2 + \mathcal{O}(\gamma^2)$ . Assuming (without loss of generality) that  $\gamma > 0$ , we notice that although the state  $u(x) = u_+$  is deterministically linearly stable, it still loses stability in the stochastically perturbed system, and the only stable state (in the limit of small noise, of course) is  $u = u_-$ . Nucleation in this system is the means of switching from the meta-stable  $u = u_+$  state to the stable  $u = u_-$  state and proceeds via the creation of a nucleus — a homoclinic orbit of the equation  $\delta \partial_{xx}^2 - 1/\delta V'(u) = 0$ . The reason that a transition occurs in this particular way is that this is the configuration with the smallest energy, small perturbations of which cause deterministic switching via the formation of two travelling waves moving away from each other. Moreover it is not hard to find that, as  $\gamma \rightarrow 0$ , the homoclinic orbit becomes a combination of a kink and antikink separated by the distance diverging logarithmically to infinity as  $\delta \ln(\gamma/8)(1 + \mathcal{O}(\gamma))/\sqrt{2}$ . This implies that, as long as  $\gamma$  scales polynomially in  $\delta$ , the size of the nucleus can be made to go to 0 as  $\delta \rightarrow 0$ . At the same time, since the space-time window  $(L, T)$  scales as  $L^2 = \mathcal{D}T$ , where  $\mathcal{D} = \mathcal{O}(\epsilon\delta)$  is the diffusion coefficient for the stochastic kink motion, taking  $\gamma = \mathcal{O}(\epsilon\delta/L)$  we will never notice the deterministic drift caused by the tilt in the potential, thus effectively remaining in the equal wells situation. The nucleation rate<sup>18</sup>  $\Theta$  can be estimated as  $\exp\{-2\mathcal{E}_k/\epsilon\}$ , where  $\mathcal{E}_k$  is the energy of one kink. Let us mention that an extensive phenomenological study of nucleation was undertaken by M. Büttiker et al. [6], [7], [8], [12]. Another discussion from the point of view of stochastic dynamical systems can be found by M. Cassandro, E. Olivieri and P. Picco [11].

**Ballistic annihilation.** In the scaling limit when the boundary layers are not pinned anymore, but are the travelling wave solutions, the limiting dynamics is not a simple diffusion process as (3.11), but a combination of both diffusion and drift

$$\dot{\zeta}_i = \pm c + \left(\frac{\mathcal{D}}{2}\right)^{\frac{1}{2}} \xi_i(t), \quad c = 3\gamma/2 + \mathcal{O}(\gamma^2), \quad \mathcal{D} = \frac{3\sqrt{2}}{2} \epsilon\delta. \quad (\text{A.1})$$

---

<sup>18</sup>Nucleation rate is the probability density that a nucleation occurs in a small space-time interval.

Plus or minus appear depending on whether the particle represents a kink or an anti-kink. Let us notice that since the scaling for the ballistic drift part is  $L = cT$ , in the asymptotic limit we will always either observe only diffusion or drift<sup>19</sup>. Considering the case when the drift is much larger than the diffusion we end up with an ensemble of particles moving with constant velocities towards (or away from) each other and annihilating mutually upon collision. This process is called **ballistic annihilation** and has been thoroughly studied by J. Piasecki [31]. It turns out to have an intrinsic relation to the statistical properties of the Burgers equation with random initial conditions which was analysed by L. Frachenbourg and P. A. Martin [20] and J. Bertoin [4].

Anomalous relaxation. In the regime of ballistic annihilation, statistical equilibrium state is achieved when the entire field is localized near the lower potential well (backward nucleation is ineffective). An interesting question appears when one asks what is the **relaxation rate**, i. e., the proportion of the field which has switched to the stable state by some time  $t$  given that we started with the entire field in the meta-stable state.

The answer is surprisingly simple for the tilted Allen-Cahn equation. Indeed in order for the field to switch at some particular point by the time  $t$  there should have been a nucleation in the space-time triangle with the area  $2cT^2$ . The probability of such nucleation is nothing else than  $1 - \exp\{-2ct^2/\Theta\}$  which yields an anomalous relaxation law. This argument is in agreement with the heuristic observations in [18]. Let us mention that the evidence of the anomalous relaxation in a biased voters model was found in [29].

Nucleation and diffusion-annihilation. We can modify equations (4.9) for diffusion-annihilation in order to account for the nucleation process. Nucleation can be treated as an additional Poisson process on the spin lattice, i. e., the spins switch their orientation with rate  $\Theta$ . In this case the diffusion coefficient  $D$  has to be changed into  $D + \Theta$  and the following terms should be added<sup>20</sup> to the right hand side of (4.9):

$$\begin{aligned} & \Theta \left[ - \left( 3 + z_k - z_1 \right) \varrho^{(k)} + \sum_{z=-\infty}^{z_1-2} \varrho^{(k)}(z, z_2, \dots) + \sum_{z=z_k+2}^{\infty} \varrho^{(k)}(\dots, z_{k-1}, z) \right. \\ & + \delta_{z_1, z_2-1} \sum_{z=-\infty}^{z_2-2} \varrho^{(k-1)}(z, z_3, \dots) + \delta_{z_k, z_{k-1}+1} \sum_{z=z_{k-1}+2}^{\infty} \varrho^{(k-1)}(\dots, z_{k-2}, z) \\ & \left. + \sum_{i=1}^{k-2} \delta_{z_i, z_{i-1}+1} \varrho^{(k-2)}(\dots, z_{i-1}, z_{i+2}, \dots) \right]. \end{aligned} \quad (\text{A.2})$$

---

<sup>19</sup>Unless  $\gamma = \mathcal{O}(\epsilon\delta/L)$  in which case the two effects can interplay.

<sup>20</sup>Equations for  $\varrho^{(1)}$  and  $\varrho^{(2)}$  require additional modifications which we do not consider here.

APPENDIX B  
**Collisional patterns of coalescing Brownian motions**

As we saw before, the question of whether some Brownian motions have or have not coalesced during a certain time naturally arises as an auxiliary problem in the context of domain-length distributions. In this section we will give a detailed analysis of this problem, following partially and improving on the treatment by B. Derrida and R. Zeutak [13]. Let us consider  $k$  point particles on the line with ordered coordinates  $x_1 \leq \dots \leq x_k$ . The particles undergo independent identical Brownian motions  $dx_i = \sqrt{\mathcal{D}/2} dB_i$ . The first question we address is the probability  $\mathcal{C}_t^{(k)}[\xi_1|\xi_2|\dots|\xi_k]$  that initially starting at locations  $\xi_i$ , no particles have collided by the time  $t$ . Denoting the probability density to observe particles at respective locations at time  $t$  (with none of them collided before) by  $\rho^{(k)}(\mathbf{x}, t)$ , we get an equation

$$\partial_t \rho^{(k)} = \mathcal{D} \Delta^{(k)} \rho^{(k)} \tag{B.1}$$

with absorbing (zero) boundary conditions at  $x_i = x_{i+1}$  and with the initial condition  $\rho^{(k)}(\mathbf{x}, 0) = \delta(\mathbf{x} - \boldsymbol{\xi})$ . Then

$$\mathcal{C}_t^{(k)}[\xi_1|\dots|\xi_k] = \int_{\mathbb{D}[12\dots k]} \dots \int \rho^{(k)}(\mathbf{x}, t) d^k \mathbf{x}, \tag{B.2}$$

where by  $\mathbb{D}[12\dots k]$  we denote the region in  $\mathbb{R}^k$  with  $x_1 < \dots < x_k$ . Although  $\rho^{(k)}(\mathbf{x})$  is only defined in  $\mathbb{D}[12\dots k]$ , let us extend its definition onto the entire space  $\mathbb{R}^k$  by simple antisymmetric reflections about the planes  $x_i = x_j$ . Such a procedure gives us a function which is completely antisymmetric with respect to any permutation of variables and which automatically provides the requested boundary conditions. Now, we can solve (B.1) in the entire space  $\mathbb{R}^k$  (of course, the probabilistic interpretation is still only valid in the original domain). In this manner the entire space initial ‘probability density’ is

$$\rho_0^{(k)}(\mathbf{x}) = \sum_{\sigma} \epsilon(\sigma) \prod_{i=1}^k \delta(x_i - \xi_{\sigma_i}), \tag{B.3}$$

where the sum is taken over all permutations  $\sigma$  of  $\{1, \dots, k\}$  and  $\epsilon(\sigma)$  is signature of the corresponding permutation. This expression is nothing other than the determinant of the matrix with entries  $\delta(x_i - \xi_j)$ . The solution to (B.1) can now be easily obtained by using Green’s function for the entire space

$$\rho^{(k)}(\mathbf{x}, t) = \int_{\mathbb{R}^k} G^{(k)}(\mathbf{y} - \mathbf{x}, t) \rho_0^{(k)}(\mathbf{y}) d^k \mathbf{y}, \tag{B.4}$$

$$G^{(k)}(\mathbf{x}, t) = \frac{1}{(4\pi\mathcal{D}t)^{k/2}} \exp\left\{-\frac{|\mathbf{x}|^2}{4\mathcal{D}t}\right\}.$$



Substituting (B.3), we compute

$$\begin{aligned}\rho^{(k)}(\mathbf{x}, t) &= \sum_{\sigma} \epsilon(\sigma) \prod_{i=1}^k \int_{-\infty}^{+\infty} G^{(1)}(y_i - x_i, t) \delta(y_i - \xi_{\sigma_i}) dy_i \\ &= \sum_{\sigma} \epsilon(\sigma) \prod_{i=1}^k G^{(1)}(x_i - \xi_{\sigma_i}, t)\end{aligned}\tag{B.5}$$

which is just an antisymmetric superposition of independent Brownian motions.

An important consequence of the antisymmetry of  $\rho^{(k)}$  is that the integrals in (B.2) may be decoupled. Indeed, let us consider all possible permutations of  $\{1, \dots, k\}$  such that the mutual ordering within the sets of indices  $\{k-1, k\}$  and  $\{1, 2, \dots, k-2\}$  is preserved. The integrals of  $\rho^{(k)}$  over the corresponding domains differ only by a sign, which depends on the signature of the permutation. It is not hard to see that by summing up all these integrals we obtain  $[k/2] \mathcal{C}_t^{(k)}[\xi_1 | \dots | \xi_k]$ , where  $[k/2]$  is the integer part of  $k/2$ . On the other hand, this sum is nothing more than

$$\int \dots \int_{\mathcal{D}[12\dots k-2]} \iint_{\mathcal{D}[k-1, k]} \rho^{(k)}(\mathbf{x}, t) d^k \mathbf{x}.\tag{B.6}$$

By iterating this procedure taking into account the oddness of  $k$ , we find the following expressions

$$\begin{aligned}\mathcal{C}_t^{(2n)}[\xi_1 | \dots | \xi_{2n}] &= \frac{1}{n!} \iint_{\mathcal{D}[1, 2]} \dots \iint_{\mathcal{D}[2n-1, 2n]} \rho^{(k)}(\mathbf{x}, t) d^k \mathbf{x} \\ \mathcal{C}_t^{(2n+1)}[\xi_1 | \dots | \xi_{2n+1}] &= \frac{1}{n!} \iint_{\mathcal{D}[1, 2]} \dots \iint_{\mathcal{D}[2n-1, 2n]} \int_{\mathcal{D}[2n+1]} \rho^{(k)}(\mathbf{x}, t) d^k \mathbf{x}.\end{aligned}\tag{B.7}$$

This decoupling allows us to express the  $k$ -particle non-collision probabilities by using only those for 2 particles, which are obtained trivially

$$\begin{aligned}\mathcal{C}_t^{(2)}[\xi_i | \xi_j] &= \iint_{\mathcal{D}[i, j]} \left[ G^{(1)}(x_i - \xi_i) G^{(1)}(x_j - \xi_j) - G^{(1)}(x_i - \xi_j) G^{(1)}(x_j - \xi_i) \right] dx_i dx_j \\ &= \operatorname{erf} \left( \frac{\xi_j - \xi_i}{\sqrt{8\mathcal{D}t}} \right), \quad \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} dy.\end{aligned}\tag{B.8}$$

By substituting solution (B.5) into (B.7), and integrating we compute

$$\begin{aligned}\mathcal{C}_t^{(k)}[\xi_1 | \dots | \xi_{2n}] &= \frac{1}{2^n n!} \sum_{\sigma} \epsilon(\sigma) \prod_{i=1}^n \mathcal{C}_t^{(k)}[\xi_{\sigma_{2i-1}} | \xi_{\sigma_{2i}}] \\ \mathcal{C}_t^{(k)}[\xi_1 | \dots | \xi_{2n+1}] &= \frac{1}{2^n n!} \sum_{\sigma} \epsilon(\sigma) \prod_{i=1}^n \mathcal{C}_t^{(k)}[\xi_{\sigma_{2i-1}} | \xi_{\sigma_{2i}}].\end{aligned}\tag{B.9}$$

Notice that in the second formula for  $k = 2n + 1$ , the sum is taken over all permutations of  $2n + 1$

indices. We can also write a formula giving recursive expressions

$$\mathcal{C}_t^{(k)}[\xi_1 | \dots | \xi_k] = \frac{1}{2^{\lfloor k/2 \rfloor}} \sum_{j=1}^{k'} (-1)^{i+j+1} \mathcal{C}_t^{(2)}[\xi_i | \xi_j] \mathcal{C}_t^{(k-2)}[\dots \xi'_i \dots \xi'_j \dots], \quad (\text{B.10})$$

where the prime near the summation sign means  $j \neq i$ , and in the second collisional configuration the particles starting at  $\xi_j$  and  $\xi_i$  are not taken into account.

Let us recall the quantities  $\mathcal{C}_t^{(k)}[\dots | \xi_m; \xi_{m+1} | \dots]$  and  $\mathcal{C}_t^{(k)}[\dots | \xi_m \xi_{m+1} | \dots]$ , which differ from  $\mathcal{C}_t^{(k)}[\xi_1 | \dots | \xi_k]$  in that in the first case we do not care whether the particles starting at  $\xi_m$  and  $\xi_{m+1}$  have collided or not, whereas in the second case we want them to have collided. First, we notice that

$$\mathcal{C}_t^{(k)}[\dots | \xi_m; \xi_{m+1} | \dots] = \mathcal{C}_t^{(k)}[\dots | \xi_m | \xi_{m+1} | \dots] + \mathcal{C}_t^{(k)}[\dots | \xi_m \xi_{m+1} | \dots]. \quad (\text{B.11})$$

The second observation is that because the Brownian motions governing the particles are independent,

$$\mathcal{C}_t^{(k)}[\dots \xi_{m-1} | \xi_m; \xi_{m+1} | \xi_{m+2} \dots] = \frac{\mathcal{C}_t^{(k)}[\dots \xi_{m-1} | \xi_m | \xi_{m+2} \dots] \mathcal{C}_t^{(k)}[\dots \xi_{m-1} | \xi_{m+1} | \xi_{m+2} \dots]}{\mathcal{C}_t^{(k)}[\dots \xi_{m-1} | \xi_{m+2} \dots]}, \quad (\text{B.12})$$

i. e., the probability that neither the  $m$ -th nor the  $(m+1)$ -st particle have collided with the rest is simply the product of the respective probabilities (this statement of course refers to the probabilities conditioned on the particular collisional pattern of the rest of the particles, which is the reason why the additional term appears in the denominator). By combining the last two formulas, we find the expression (shortening notation down to the indices alone)

$$\mathcal{C}_t^{(k)}[\dots 1 | 23 | 4 \dots] = \frac{\mathcal{C}_t^{(k-1)}[\dots 1 | 2 | 4 \dots] \mathcal{C}_t^{(k-1)}[\dots 1 | 3 | 4 \dots]}{\mathcal{C}_t^{(k-1)}[\dots 1 | 4 \dots]} - \mathcal{C}_t^{(k)}[\dots 1 | 2 | 3 | 4 \dots]. \quad (\text{B.13})$$

By applying the same procedure to ‘decouple’ all the entries, we can obtain explicit expressions for all quantities  $\mathcal{C}_t^{(k)}[1 | 23 | 45 | \dots | n - 2n - 1 | n]$ , which give the inter-particle probability densities for the diffusion-coalescence process (4.25).

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