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Dynamical Gibbs-non-Gibbs transitions: a study via coupling and large deviations

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Dynamical Gibbs-non-Gibbs transitions: a study via coupling and large deviations

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Feijia Wang

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Beoordelingscommissie:	Prof. dr. A.C.D. van Enter
	Prof. dr. C. Külske
	Dr. A. Le Ny

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1

Introduction

Statistical mechanics studies the collective statistical properties of a system composed of a large number of components. The components could, for instance, be particles (in lattice gas systems, see e.g. Chapters 1–2 of [1] and references therein), (magnetic) spins (in spin systems for ferromagnets, e.g. the *Ising model* [32]), pixels (in image analysis [23]), economic agents (in economics [20]), etc. This thesis focuses on the spin interpretation of the components. The spins are usually labeled by vertex sets of some underlying (finite/infinite) graph, whose connectivity structure determines the interdependence among the spins. Among the graphs that have been considered in the literature are the d-dimensional integer lattice and the complete graph. The system on the lattice is called lattice-spin system. Here the underlying geometry of the lattice plays a crucial role. The case on the complete graph is referred to as a mean-field spin system. Here there is no geometry.

In equilibrium statistical mechanics, such a study begins by prescribing a *Hamiltonian*[1] H that associates to each microscopic description (*configuration*) σ of the system an energy. Usually H comes with several parameters such as temperature, external field, chemical potential etc. depending on the system under consideration. Given an H, the equilibrium behavior of the system is modeled by the Gibbs probability measure μ on the configurations that takes the form, in finite volume,

$$\mu(\sigma) \propto e^{-H(\sigma)}. \tag{1.0.1}$$

In the thermodynamic limit, e.g., on the full lattice $\mathbb{Z}^d$, formula (1.0.1) does no longer make sense. To give meaning to H, one measures the energy H_Λ^ζ of the system in a finite window Λ of the lattice when everything outside the window is fixed to a configuration ζ. Thus for any pair of Λ and ζ, the associated *finite-volume Gibbs measure*

$$\mu_\Lambda^\zeta(\sigma) \propto e^{-H_\Lambda^\zeta(\sigma)} \tag{1.0.2}$$

[1] Formal definitions of terms will be in Subsection 1.2.1.

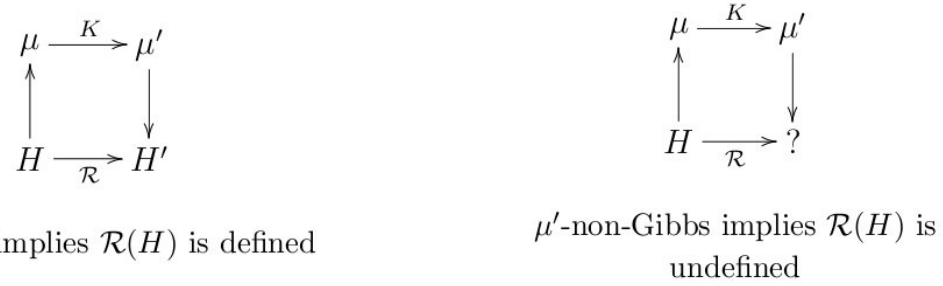

Figure 1.1: Diagram of renormalization group transformation

(the *Boltzmann-Gibbs distribution*) describes the equilibrium behavior of the system in Λ when everything outside Λ is set to ζ. The family γ of all finite-volume Gibbs measures μ_Λ^ζ is said to be a *Gibbs specification* if μ_Λ^ζ is "continuous (quasilocal)"as a function of ζ. A probability measure μ on the configurations is a *Gibbs measure* associated with H if it has γ as a version of its conditional distributions. The relations (1.0.2) are referred to as the *DLR equations*, after Dobrushin [8, 9], Lanford and Ruelle [37] who introduced them in the 1960s. There can be one or more Gibbs measures associated with the Gibbs specification γ. The non-uniqueness of Gibbs measures indicates the occurrence of a *first-order phase transition*, such a transition accompanied with the presence of spontaneous magnetization, and uniqueness is an indication of the lack of a first-order phase transition. For more background on Gibbs measures, we refer the reader to [13, 19, 24, 39]. In what follows we say that a spin system is Gibbsian if it has a Gibbs measure describing its equilibrium behavior.

The main question that laid the basis of an area of research is whether a transformed Gibbsian spin system will remain Gibbsian. This question originated from the study of renormalization group transformations, a technique for studying phase transitions and critical phenomena. A renormalization group transformation $\mathcal{R}$ is a map from the space of Hamiltonians onto itself. For such a map to be useful it has to be well defined. But as Griffiths and Pearce [27, 28] pointed out in the late 1970's, there is a serious problem when it comes to precisely defining the map $\mathcal{R}$. The map $\mathcal{R}$ on Hamiltonians H naturally induces a map K that associates to each Gibbs measure μ of H a renormalized probability measure $\mu' = K\mu$. R.B. Israel [33] noted after this observation that the question of whether $H' = \mathcal{R}H$ is well-defined is directly linked to the the problem of whether μ' is Gibbs or not. If μ' is a Gibbs measure then H' exists and H' does not exist otherwise (see Figure 1.1). This gave rise to a surge of activity in trying to identify when a renormalized Gibbs measure retains or loses its Gibbs property. Renormalization maps that have been studied in the literature include decimation, block-spin, Kadanoff transformations, etc. [13, 19, 39].

Other forms of transformations K, such as stochastic time-evolution or coarse-graining of the spin space, have been applied to Gibbs measures of various lattice and mean-field systems. In all these cases, the Gibbs property is sometimes retained and sometimes lost [11, 14, 16, 17, 21, 30, 40]. In particular in the paper by van Enter, Fernandez, den Hollander and Redig [11] it was shown that in an independent spin-flip dynamics of Ising spins starting from an Ising Gibbs measure below the critical temperature the system will remain Gibbs in a short interval of time and then becomes non-Gibbs at large enough times. This loss of the Gibbs property persists at all later times if the initial Ising model has zero external magnetic field. However, the Gibbs property is restored at large but finite later times in the case of a small positive initial external magnetic field.

The proof of whether the transformed measure μ' is Gibbs or not consists of checking if the conditional distributions of μ' have the quasilocality property or not. The loss of the quasilocality property is associated with a phase transition in a so-called 'constrained system'. This constrained system is obtained as follows: Consider the joint distribution $\bar{\mu}$ of the original (initial) spins σ and the transformed spins ξ. For a fixed transformed configuration ξ, the law, under $\bar{\mu}$, of the initial spins σ that are mapped to ξ by the transformation K is what we called the constrained system. The joint measure $\bar{\mu}$ is also called the two-layer system. The transformed measure μ' is Gibbs if for every fixed transformed configuration ξ, the associated constrained system has a unique Gibbs measure, and it becomes non-Gibbs otherwise. A ξ configuration is said to be *bad* for μ' if the associated constrained system undergoes a phase transition and *good* otherwise.

In the case where K is a stochastic time-evolution transformation, the two-layer system describes what happens to the system at only two different times, namely what happens at time zero and at time $T > 0$. This has led to a large deviation approach to the study of dynamical Gibbs-non-Gibbs transitions. This approach looks at the large deviation properties of random paths that are generated by the time-evolution of some random variables that are derived from the configurations of the system under consideration. For lattice spin systems the observable of interest is the empirical measure of the configurations. In the mean-field set-up the empirical distribution of the configuration is the preferred observable. For mean-field models with binary spins the empirical average is used since in this case the empirical distribution and empirical average contain the same information. The idea here is to study the optimal trajectories (minimizers of the large deviation rate function) for the large deviation rate functional for the law of all trajectories ending at a given fixed point at time T. This law is the path-wise counterpart of the constrained system in the two-layer picture. Note that in the lattice two-layer picture we fix a configuration at time T while here we fix an empirical measure at time T. However, in the mean-field case what is fixed

in both cases is the empirical distribution. The aim is to link the existence of multiple optimal trajectories in the large deviation approach to the existence of phase transition in the constrained system in the two-layer picture. This will imply that the transformed measure μ' is non-Gibbs if there are multiple optimal trajectories and is Gibbs otherwise. Thus in the large deviation approach to lattice spin systems we speak of bad empirical measure instead. This link has been established for the mean-field Curie-Weiss Ising model under independent spin-flip dynamics by V. Ermolaev and C. Külske [17], R. Fernández, F. den Hollander and J. Martinez [21] and A. Le Ny and C. Külske [34]. In fact in this particular case the two approaches are equivalent. In the lattice set-up the proposal is to show that every typical configuration of a bad empirical measure is a bad configuration. This program has been pioneered by A. van Enter, R. Fernández, F. den Hollander and F. Redig [12].

The focus has always been checking whether a transformed Gibbs measure is Gibbs or not. In the case the transformed measure μ' is Gibbs, one may like to know other properties of μ' such as, the associated transformed Hamiltonian H', decay of spatial correlations etc. These issues have not been well addressed in the literature. To our knowledge, the only results for the decay of the potential of the transformed measure are found in [35, 41, 42, 43, 44, 45].

1.1 Overview of thesis

In this thesis we study the conservation and loss of the Gibbs property for both lattice and mean-field spin systems. We use both the two-layer and the large deviation approaches. Let us now review the main results of the thesis leaving the technical details to the body of the thesis.

1.1.1 Conservation of Gibbsianness for lattice spin systems

Chapter 2 of the thesis studies the transforms of one-dimensional lattice spin systems. We start from a Gibbs measure with infinite range interaction, i.e., the Hamiltonian of the initial system need not be of finite range but has to admit a unique Gibbs measure. We consider both deterministic and stochastic transformations K. They do not need to be applied independently at the sites. Using the two-layer approach we prove that the constrained system has a unique Gibbs measure for every choice of transformed configuration, as long as the range of K is finite. This implies that the associated transformed Gibbs measures are always Gibbs. Note that for stochastic transformations the constrained system has a full support while their deterministic counterparts are supported on subspaces of the

initial configuration space. Further, we provide information about the spatial decay of the transformed potential. In particular, if the initial interaction is exponentially decaying, then the transformed interaction decays exponentially as well. If the initial interaction decays as a power law with power α (which is chosen big enough to be in the uniqueness regime), then the transformed interaction can be estimated with a (smaller) power as well.

The proofs of these results use the *house-of-cards coupling* argument from [2]. This coupling exploits the fact that the dimension of the lattice is one.

1.1.2 Dynamical Gibbs-non-Gibbs transitions for mean-field spin systems

New and explicitly computable examples of Gibbs-non-Gibbs transitions for mean-field continuous spin systems are studied by using the large deviation approach in Chapter 3 of the thesis. The starting mean-field measure μ_n^F on a complete graph with $n \in \mathbb{N}$ vertices takes the form

$$\mu_n^F(dx_1, \cdots, dx_n) = \frac{1}{Z_n^F} e^{nF\left(\frac{1}{n}\sum_{i=1}^n x_i\right)} \prod_{i=1}^n \alpha(dx_i), \tag{1.1.1}$$

where α is the standard Gaussian distribution, Z_n^F is the normalizing partition sum,

$$F(y) = \frac{y^2}{2} - G(y), \tag{1.1.2}$$

and G is a continuously differentiable function. This measure only looks at the empirical average $\overline{x}_n = (1/n)\sum_{i=1}^n x_i$ of the spin configuration. Therefore one can look at μ_n^F as a probability measure on the empirical average $\overline{x}_n$.With the above choice of F, μ_n^F is Gibbs in the mean-field sense [34, 36]. We then study the Gibbs-non-Gibbs properties (in the mean-field sense) of μ_n^F subjected to various forms of dynamics. For the purpose of the discussion here we choose the "the double-well potential"

$$G(y) = (y^2 - a^2)^2, \tag{1.1.3}$$

where $a > 0$. In Chapter 3 other forms of G are considered as well.

Independent Brownian motions

First we consider independent standard Brownian motions on $\mathbb{R}$ indexed by the vertices of the complete graph K_n starting from the mean-field measure μ_n^F. At the level of the empirical average this dynamics corresponds to a Brownian motion with small variance (average of n independent Brownian motions). With this dynamics and the above choice of G we prove that there is a critical time T_{crit} with

$$T_{crit} = \frac{1}{4a^2}, \tag{1.1.4}$$

such that

$$\begin{cases} \text{there is a unique optimal trajectory if } T \leq T_{crit} \\ \text{there are multiple optimal trajectories if } T > T_{crit}, \end{cases}$$

and that there is only one bad empirical average $b = 0$ when $T > T_{crit}$. Here the "badness"is in the following sense. $\{m_n(t)\}_{n\in\mathbb{N}}$ denoting a sequence of stochastic processes for the empirical average, we say that a point $b \in \mathbb{R}$ is a *bad* at time T if the following two conditions hold:

1. Conditional on $m_n(T) = b$, $m_n(0)$ does not converge (as $n \to \infty$) to a point-mass in distribution.

2. There exist two sequences $b_k^+ \to b$, $b_k^- \to b$ and $\delta > 0$ such that the variational distance between the distribution $\mu(0, T; b_k^+)$ of $m_n(0)|m_n(T) = b_k^+$ and the distribution $\mu(0, T; b_k^-)$ of $m_n(0)|m_n(T) = b_k^-$ is at least δ for k large enough.

Thus T_{crit} is the time before which the transformed measure μ'_T is Gibbs and after which it is non-Gibbs, where Gibbs/non-Gibbs is in the mean-field sense originally introduced in [34]. Up to time T_{crit} all empirical averages are good and after T_{crit}, $b = 0$ becomes the only bad empirical average. The above result extends to Brownian motions with constant drift V. In this general context the critical time remains the same and after the critical time there is a time-dependent bad empirical average b. This is unique for each time instance and is given by $b = VT$, for any $T > T_{crit}$.

Ornstein-Uhlenbeck process

Second we apply an Ornstein-Uhlenbeck dynamics to the empirical average with μ_n^F as the starting distribution.

Then the time-evolved measure μ'_T is the projection at time T of the law of the solution to the stochastic differential equation

$$dX_t^n = (-\kappa X_t + E)dt + \frac{1}{\sqrt{n}} dB_t, \tag{1.1.5}$$

where κ and E are real-valued parameters and B_t is the standard Brownian motion. This is a generalization of the previous dynamics in the sense that here we consider non-constant drift. Under this dynamics we have a critical time

$$T_{crit} = \frac{1}{2\kappa} \log\left(1 + \frac{\kappa}{2a^2}\right) \tag{1.1.6}$$

below and on which there is always a unique optimal trajectory, i.e. the time evolved measure is Gibbs and above which there are multiple trajectories associated with the time dependent bad empirical average

$$b = \frac{E}{\kappa}(1 - e^{-\kappa T}). \tag{1.1.7}$$

At any time instance beyond T_{crit}, the b above is the only bad empirical average.

If the drift term $-\kappa X_t + E$ in (1.1.5) is replaced by a general drift term $f(X_t)$, where f is an odd function and satisfies some other regularity conditions, then we can also show that for short times the time evolved measure is Gibbs and becomes non-Gibbs at later times. We have in this case no explicit expression for the critical time but we know the empirical average $b = 0$ is bad (possibly other bad configurations can exist in this case).

Birth and death process

Further, we consider birth and death dynamics of the empirical average starting from μ_n^F, i.e., we consider a continuous time random walk X_t^n on $\mathbb{R}$ with initial distribution μ_n^F which makes jumps of size $\pm 1/n$ at rates $nb(x)$, resp. $nd(x)$. For constant birth and death rates b and d, we obtain the same results as in the case of Brownian motion with constant drift. Note that the case we choose the birth and death rates to $b(x) = \gamma(1-x)$ and $d(x) = (1+x)$, with $x \in [-1, 1]$ and $\gamma \geq 1$, corresponds to the independent spin-flip dynamics (with an external field) of the empirical average of Ising spins. In this case we obtain, by analogy with the case of the Ornstein-Uhlenbeck process, that at short time the system stays Gibbs and becomes non-Gibbs at later time with time dependent bad empirical average

$$b = \frac{\gamma - 1}{\gamma + 1}\left(1 - e^{-(1+\gamma)T}\right). \tag{1.1.8}$$

Here, contrary to the Ornstein-Uhlenbeck case, we have no explicit expression for the critical time.

The proofs of the above results use the Feng-Kurtz scheme [12, 18] to obtain a path-wise large deviation rate functional for the constrained system. The optimal trajectories are then obtained by minimizing this functional.

The rest of the thesis is organized as follows: In the rest of this chapter we collect the tools that are used in the rest of the thesis. Chapter 2 contains the results for transforms of one-dimensional Gibbs measures. The results on the dynamical Gibbs-non-Gibbs transitions for mean-field spin system are found in Chapter 3.

1.1.3 Large deviations for the trajectory of the empirical distribution and empirical measure

In Chapter 4 we compute the Feng-Kurtz Hamiltonian and Lagrangian associated to the large deviations of the trajectory of the empirical distribution for independent Markov processes, and of the empirical measure for translation invariant interacting Markov processes. We treat both the case of jump processes (continuous-time Markov chains and interacting particle systems) as well as diffusion processes. For diffusion processes, the Lagrangian is a quadratic form of the deviation of the trajectory from the Kolmogorov forward equation. In all cases, the Lagrangian can be interpreted as a relative entropy (density) per unit time.

1.2 Generalities on Gibbs and non-Gibbs measures

This section contains generalities on Gibbs and non-Gibbs measures. For more background on Gibbs and non-Gibbs measures we refer the reader to [13, 19, 24, 39].

1.2.1 Gibbs measures

Let S be the single-site space, i.e. the set of all possible values for a spin. We assume S is a Polish space and is equipped with the Borel sigma algebra $\mathcal{S}$ associated with the topology on S. Mostly we consider S to be $\{-1, 1\}$, a finite set, $\mathbb{R}$ or an interval. Turn S into a measure space by equipping it with an a priori measure ρ, usually a probability measure. Denote by $\Omega = S^{\mathbb{Z}^d}$ the spin configuration space, describing all possible microscopic state of the system, where $\mathbb{Z}^d$ is the d-dimensional integer lattice with $d \geq 1$. Equip Ω with the product topology and the product sigma algebra $\mathcal{F} = \mathcal{S}^{\mathbb{Z}^d}$. In what follows we will use upper case Latin and Greek letters to represent subsets of $\mathbb{Z}^d$ and lower case Latin and Greek letters to denote elements in Ω.

For any subset $\Lambda \subseteq \mathbb{Z}^d$, denote by $\mathcal{F}_\Lambda$ the sigma algebra generated by the spins in Λ. Denote by $\mathcal{L}$ the set of all finite subsets of $\mathbb{Z}^d$. For $\sigma \in \Omega$ and $\Lambda \in \mathcal{L}$, we denote by σ_Λ the restriction of σ to Λ. A bounded measurable function $f : \Omega \to \mathbb{R}$ is called *local* if there exists some $\Delta \in \mathcal{L}$ such that f is $\mathcal{F}_\Delta$-measurable. The function f is said to be *quasilocal* if it is a uniform limit of local functions.

Potential and Hamiltonian

Definition 1.2.1. *A potential is a function $\Phi : \mathcal{L} \times \Omega \to \mathbb{R}$ such that $\Phi(\Lambda, .)$ is $\mathcal{F}_\Lambda$-measurable ($\Phi(\Lambda, .) \in \mathcal{F}_\Lambda$) for all $\Lambda \in \mathcal{L}$. A potential Φ is called uniformly absolutely*

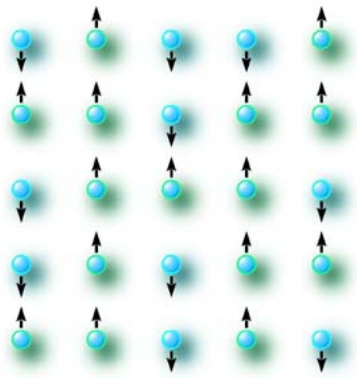

Figure 1.2: Ising model, the most well-known lattice-spin model, on a 2-dimensional lattice

convergent (UAC) if for all $x \in \mathbb{Z}^d$

$$\sum_{A \ni x} \|\Phi(A,\sigma)\|_\infty < \infty, \tag{1.2.1}$$

where $\|\Phi(A,\sigma)\|_\infty = \sup_{\sigma\in\Omega} |\Phi(A,\sigma)|$.

Example 1.2.1. The family Φ given by

$$\Phi_A = \begin{cases} -J\sigma_x\sigma_y & \text{if } |x-y| = 1 \text{ and } A = \{x,y\} \\ -h\sigma_x & \text{if } x = y \\ 0 & \text{otherwise,} \end{cases} \tag{1.2.2}$$

where $S = \{-1,+1\}$ and $J > 0$, $h \in \mathbb{R}$. J is called the interaction strength and h is the external magnetic field. This interaction gives rise to the *Ising model* [32] for *ferromagnetism*. It is one of the most studied statistical mechanical models. This is a lattice spin model for studying the phenomenon of ferromagnetism, i.e. it is a model for studying why at low temperatures a piece of iron metal will continue to be magnetized even after a source of external magnetic field that it was in contact with is withdrawn. This phenomenon was believed to be associated with the alignment of the magnetic moments of the atoms. The Ising model is a very simplified model where a magnetic moment is allowed to take two different directions, namely it can point up $(+1)$ or down (-1). See Figure 1.2 for an example of an Ising spin configuration in two dimensions. Note that the Ising potential is also UAC.

Definition 1.2.2. *For* $\zeta \in \Omega$ *and* $\Lambda \in \mathcal{L}$*, the finite-volume Hamiltonian corresponding to potential* Φ *and with boundary condition* ζ *is defined as*

$$H_\Lambda^{\Phi,\zeta}(\sigma) = \sum_{A \bigcap \Lambda \neq \varnothing} \Phi(A, \sigma_\Lambda \zeta_{\Lambda^c}), \quad \sigma \in \Omega, \tag{1.2.3}$$

where $\sigma_\Lambda\zeta_{\Lambda^c}$ *is the configuration in* Ω *that coincides with* σ *on* Λ *and coincides with* ζ *on* Λ^c.

Remark 1.2.1. Note that $H_\Lambda^{\Phi,\zeta}$ is well-defined and is quasilocal as a function of ζ if Φ is UAC.

Finite/infinite-volume Gibbs measures and the DLR equations

Definition 1.2.3. *For any potential Φ satisfying 1.2.1 the finite-volume Gibbs measure $\mu_{\Lambda}^{\Phi,\zeta}$ associated with $\Lambda \in \mathcal{L}$, the boundary condition ζ and temperature $T = 1/\beta$ is given by*

$$\mu_{\Lambda,\beta}^{\Phi,\zeta}(d\sigma) = \frac{\exp\left(-\beta H_{\Lambda}^{\Phi,\zeta}(\sigma)\right)}{Z_{\Lambda}^{\zeta}} \prod_{i\in\Lambda} \rho(d\sigma_i), \tag{1.2.4}$$

where Z_{Λ}^{ζ} is the normalizing partition sum. The family $\gamma^{\Phi} = \{\mu_{\Lambda,\beta}^{\Phi,\zeta}, \zeta \in \Omega, \Lambda \in \mathcal{L}\}$ of finite-volume Gibbs measures is called a Gibbs specification.

Remark 1.2.2. For any UAC potential Φ, the family γ^{Φ} is quasilocal, meaning that for any bounded quasilocal function f, on Ω, and any $\Lambda \in \mathcal{L}$

$$\lim_{\Delta\uparrow\mathbb{Z}^d} \sup_{\eta,\zeta\in\Omega;} \left|\mu_{\Lambda,\beta}^{\Phi,\eta_\Delta\zeta_{\Delta^c}}(f) - \mu_{\Lambda,\beta}^{\Phi,\eta}(f)\right| = 0, \tag{1.2.5}$$

i.e. the expectation w.r.t. $\mu_{\Lambda,\beta}^{\Phi,\cdot}$ of a quasilocal function is again quasilocal, for all $\Lambda \in \mathcal{L}$.

Definition 1.2.4. *A probability measure μ on Ω is called a Gibbs measure associated with a UAC potential Φ, ρ and β if γ^{Φ} is a version of its conditional probabilities, i.e. for any $\Lambda \in \mathcal{L}$ and bounded $\mathcal{F}$-measurable function f on Ω*

$$\mu(f|\mathcal{F}_{\Lambda^c})(\cdot) = \mu_{\Lambda,\beta}^{\Phi,\cdot}(f), \quad \mu - a.s.. \tag{1.2.6}$$

The measure μ with the above property is said to be compatible with (or admitted by) γ^{Φ}.

The equations (1.2.6) are called the *DLR equations*, after Dobrushin, Lanford and Ruelle [8, 9, 37].

Existence and uniqueness of Gibbs measure

We denote by $\mathcal{G}(\gamma^{\Phi})$ the set of Gibbs measures admitted by γ^{Φ}. If the single-site space S is finite (and thus compact), its follows from the general weak convergence properties that for every net of finite-volume Gibbs measures with boundary condition has a subnet with an accumulation point. Further, if the associated specification is quasilocal, the accumulation point is a Gibbs measure by the DLR equations. This also implies that the cardinality of $\mathcal{G}(\gamma^{\Phi})$ is at least one for γ^{Φ} associated with a UAC interaction.

Next, for a quasilocal specification γ^{Φ}, the cardinality of $\mathcal{G}(\gamma^{\Phi})$ is exactly one in the following scenarios:

1. There is no interaction among the spins. This occurs when β is zero or when Φ is non-zero only for single-sites. Then the Gibbs measure is a product measure.

2. When the specification γ^Φ satisfies Dobrushin's condition, see [24] Section 8.1. In this case either there is small interaction among the spins and the Gibbs measure is a small perturbation from a product measure or there is a very strong external field.

3. For one-dimensional lattice models, if the potential Φ satisfies

$$\sum_{n=0}^{\infty} f(n) < \infty \tag{1.2.7}$$

where

$$f(K) = \sup_{i\in\mathbb{Z}} \sum_{A\ni i, diam(A)\geq K} \|\Phi(A,\sigma)\|_\infty, \tag{1.2.8}$$

then γ^Φ admits a unique Gibbs measure, see [24] Section 8.3. The one-dimensional Ising model and one-dimensional lattice-spin models with finite range interaction clearly belong to this family. The long-range Ising potential

$$\Phi(\{i,j\},\sigma) = \frac{\sigma_i\sigma_j}{|j-i|^\gamma} \tag{1.2.9}$$

also belongs to this family when $\gamma > 2$ (γ^Φ admits in fact multiple Gibbs measures when $\gamma \in (1,2]$).

Non-uniqueness of Gibbs measure

The existence of more than one Gibbs measure for γ^Φ, such as the one-dimensional long-range Ising models (1.2.9) for $\gamma \in (1,2]$ or the nearest neighbor Ising models (1.2.2) of dimension higher than one with low temperature, corresponds to the occurrence of a first-order phase transition.

Let's look at an example of γ^Φ that admits multiple Gibbs measures. The example we consider here is the γ^Φ associated with the Ising interaction (1.2.2). The one-dimensional version of this model, as we saw above, admits a unique Gibbs measure. This was the case Ising treated in his PhD. Thesis. The original goal of Ising and his adviser Lenz was to show that at low temperatures the magnetization of their model as a function of the external field h behaves discontinuously at $h = 0$ (*spontaneous magnetization*), i.e., at low temperatures a ferromagnetic substance will retain a net magnetization oriented in the direction of the external field it is contact with even if this external source is turned off. To the disappointment of Ising this behavior was absent in the one-dimensional case he considered and he concluded this should be the case for models in dimensions higher than one.

R.E. Peierls [46] gave an argument that disproved the claim for dimensions higher than one. This argument was later made rigorous by Dobrushin [7] and Griffiths [26]. The proof

considers the case $h = 0$. The heuristic argument behind the proof is that at low temperatures the Gibbs measures are supported on configurations that are small perturbations of the configurations that minimize the Ising Hamiltonian (ground state). For $h = 0$ there are two such configurations, namely the all plus (+1) and the all minus (-1) configurations. Therefore, if μ^+ is a Gibbs measure obtained from a weak limit along a net of elements in γ^Φ with the all plus (+1) boundary condition, then this measure will remember that it came from a net of finite-volume Gibbs measures with all plus boundary condition. That is the expected value of the spin at the origin is positive, even after taking the infinite-volume limit. Similarly, if μ^- is constructed as above from an all minus (-1) boundary condition, it will also give a negative expected value to the spin at the origin. This implies that at low enough temperatures there exist at least two Gibbs measures admitted by γ^Φ, one negatively magnetized and the other positively magnetized. For instance, the μ^+ measure lives on configurations that are a sea of +'s with islands of minuses. In the Peierls argument the sites that are of interest, as far as the Hamiltonian is concerned, are those pairs of sites with misaligned spins. These sites serve as the boundary sites for an island of minuses. Such sites determine a $(d-1)$-dimensional connected surfaces. Each such connected surface is called a *contour*. Each spin configuration corresponds uniquely (up to simultaneous flipping of all spins) to a family of contours. The Peierls argument, essentially shows that under μ^+ at low enough temperatures, the probability of having a finite contour surrounding the origin is strictly less than one-half.

1.2.2 Transformation of Gibbs measures and phenomenon of non-Gibbsianness

A probability measure μ on Ω is said to be *non-Gibbsian* if there is no UAC potential for which its conditional probabilities can be written in the form (1.2.6). This usually occurs when the conditional distributions of μ do not satisfy (1.2.5). This means that there is a so-called *bad configuration* that leads to the violation of (1.2.5). More precisely, in the case that the single-site space S is compact, it is defined as follows.

Definition 1.2.5. *A configuration $\eta \in \Omega$ is said to be bad for a probability measure μ if there exist $\epsilon > 0$ and $x \in \mathbb{Z}^d$ such that for all $\Lambda \in \mathcal{L}$, with $x \in \Lambda$, there exist $\Gamma \supset \Lambda$, with $\Gamma \in \mathcal{L}$, such that:*

$$\sup_{\xi,\zeta} \left| \mu_\Gamma(\sigma_x | \eta_{\Lambda\setminus\{x\}} \xi_{\Gamma\setminus\Lambda}) - \mu_\Gamma(\sigma_x | \eta_{\Lambda\setminus\{x\}} \zeta_{\Gamma\setminus\Lambda}) \right| > \epsilon. \tag{1.2.10}$$

This implies that η is an essential point of discontinuity of every version of the conditional probability of $\mu(\sigma_x|(\cdot)_{\mathbb{Z}^d\setminus\{x\}})$.

Non-Gibbsian measures arise naturally from transformations of Gibbs measures as was mentioned earlier in this chapter. Such transformations are usually in the form of

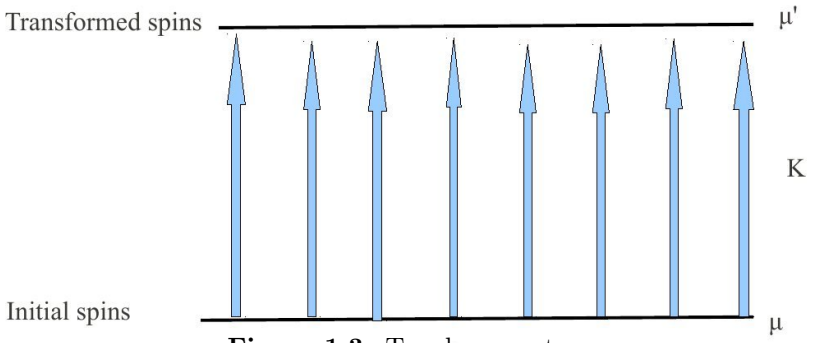

Figure 1.3: Two-layer system

1. Coarse-graining of initial lattice and projection of initial lattice to lower-dimensional lattice as is done for renormalization group (RG) transformations such as block-spin transformations, decimation transformations, Kadanoff transformations [3, 13, 27, 28, 29, 33].

2. Fuzzification or discretization of the initial spin space [14, 30, 50].

3. Stochastic time-evolution of Gibbs measures [6, 11, 15, 16, 40, 45, 47].

In all these transformations the Gibbs property of the initial system is for some times conserved and for other times lost.

1.2.3 The two-layer picture

Consider a Gibbs measure μ for an initial spin system and then generate a new probability measure μ' by applying a probability kernel K to μ,

$$\mu'(\omega') = (\mu K)(\omega') \equiv \sum_{\omega} \mu(\omega) K(\omega \to \omega'). \tag{1.2.11}$$

μ and μ' need not live on the same configuration space. To prove that the transformed measure μ' is Gibbs or not one usually considers the so-called two-layer system $\bar{\mu}$ consisting of the initial spins, that are distributed according to μ, and the transformed spins. The initial and the transformed spins are coupled together by K in such a way that the marginal of this joint distribution to the transformed spins is μ', see Figure 1.3.

The problem of checking whether μ' is Gibbs or not reduces to the problem of checking whether the constrained system $\bar{\mu}[\eta]$, i.e. the joint system constrained to configurations $\Omega_\eta \times \{\eta\}$ where Ω_η is the set of those initial spins that are mapped to η by K, exhibits phase transitions or not. If the constrained system has a unique Gibbs measure uniformly in η, then μ' is Gibbs and μ' is non-Gibbs otherwise.

Let us look at some examples.

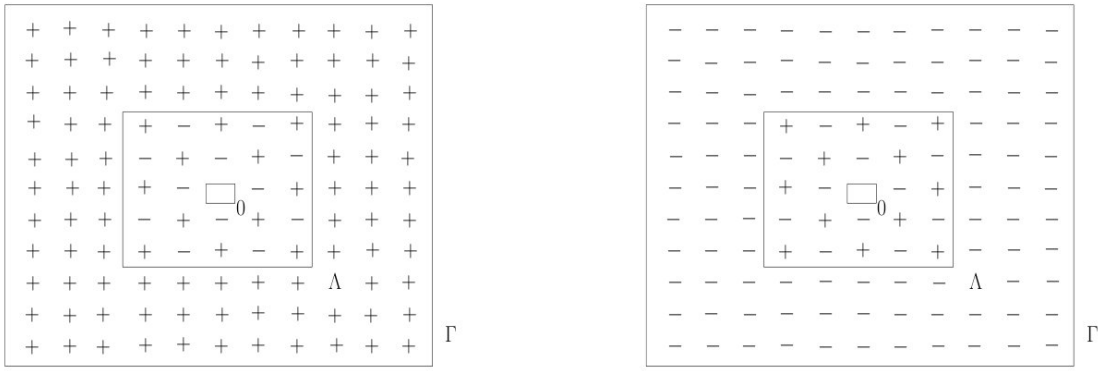

Figure 1.4: A plus-minus alternating configuration approximated with the all-plus boundary (left) and approximated with the all-minus boundary (right).

Example 1.2.2. Let μ^+ be the plus phase for the d-dimensional Ising at low enough temperature. Starting from μ^+, Van Enter, Fernandez, den Hollander and Redig [11], considered infinite/high temperature spin-flip dynamics of the initial spins towards a reversible Gibbs measure. Under this dynamics the time-evolved measure μ_t^+ was shown to be Gibbs for short times and non-Gibbs at later times. In the case there is a small positive external field the measure becomes Gibbs again at large but finite times. For the case of zero external field for the initial system the Gibbs property is lost forever.

The intuitive argument for these Gibbs-non-Gibbs transitions is as follows: The constrained system can be viewed as the initial system with a dynamical external field. This field is generated by the constraint on the second layer. For short times this field is very strong and forces the constrained system to be in the uniqueness regime. The strength of the field decays to zero as time goes to infinity. If we start with an initial system with zero external field, then at large enough times there will be configurations that are neutral with respect to the all-plus boundary and the all-minus boundary, such as a plus-minus alternating configuration (see Figure 1.4), meaning there exists a phase transition for the constrained system. On the other hand, if the initial system has non-zero initial field, we can choose the constrained second-layer configuration in such a way that in an intermediate range of times the dynamical field cancels the initial field in the constrained system. This will cause the constrained system to exhibit a phase transition if the temperature is low enough. But if we wait long enough the dynamical field will fade away giving way to the initial field to once again force the constrained system into the uniqueness regime.

Example 1.2.3. Next we consider the decimation transformation of the 2-dimensional Ising model [13, 38]. The decimation transformation K with spacing 2 maps the configuration space Ω onto itself in the following sense: For any initial configuration $\omega \in \Omega$, $\omega' = K\omega$ is such that $\omega'_x = \omega_{2x}$, for $x \in \mathbb{Z}$. Then, as before, we apply the decimation transformation to a Gibbs measure μ of a low-temperature Ising model. Note that here the transformed spins live on the even lattice $2\mathbb{Z}^2$. The two-layer system lives on $\mathbb{Z}^2$ and in this case it is the same as the

initial spin system. The constrained system associated with the transformed configuration ω' lives on $\mathbb{Z}^2$ but is supported on the configurations with all spins in $2\mathbb{Z}^2$ fixed to ω'. For an initial Ising model at low enough temperature and in zero field, the constrained system associated with a plus-minus alternating configuration (bad configuration) admits multiple Gibbs measures and the decimated measure becomes non-Gibbs. In the case we start with initial Ising model at low enough temperature and in non-zero field, it is shown that a bad configuration, different from the plus-minus alternating configuration, is needed to 'annihilate' the initial external field to force the constrained system into the phase transition regime.

1.3 Large deviation theory and optimal solutions for rate function

In this section we collect some results from the theory of large deviations. Large deviation theory deals with deviations, of certain random objects, larger than those captured by the central limit theorem.

1.3.1 Large deviation principle

Here we collect some general notions for large deviations. For more background on large deviations, we refer the reader to [5, 10, 31]. Let $\mathcal{X}$ be a Polish space, i.e. a complete separable metric space.

Definition 1.3.1. *The function $I : \mathcal{X} \mapsto [0, \infty]$ is called a rate function if*

1. *$I \neq \infty$,*
2. *I is lower semi-continuous,*
3. *I has compact level sets.*

Definition 1.3.2. *A sequence of probability measures $(P_n)_{n\in\mathbb{N}}$ on $\mathcal{X}$ satisfies the large deviation principle (LDP) with rate n and with rate function I if*

1. *I is a rate function in the sense of Definition 1.3.1,*
2. *$\limsup_{n\to\infty} \frac{1}{n} \log P_n(C) \leq -I(C) \ \ \forall C \subseteq \mathcal{X}$ closed,*
3. *$\liminf_{n\to\infty} \frac{1}{n} \log P_n(O) \geq -I(O) \ \ \forall O \subseteq \mathcal{X}$ open,*

where $I(S) = \inf_{x\in S} I(x)$ for any $S \subseteq \mathcal{X}$.

Let us now discuss some examples of sequences of probability measures that will appear in the later part of the thesis. Consider the sequence $X = (X_n)_{n\in\mathbb{N}}$ of real-valued independent and identically distributed random variables with common law ρ. The first result is Cramér's Theorem [4], for the sequence of probability measures $(P_n)_{n\in\mathbb{N}}$, where P_n is the law of the *empirical average*

$$L_n^{(1)} = \frac{1}{n}\sum_{i=1}^{n} X_i. \tag{1.3.1}$$

Theorem 1.3.3 (Cramér's Theorem). *Let P_n be as above and suppose that*

$$\varphi(t) = \int_{\mathbb{R}} e^{tx}\rho(dx) < \infty, \quad \textit{for any} \quad t \in \mathbb{R}. \tag{1.3.2}$$

Then the sequence of probability measures $(P_n)_{n\in\mathbb{N}}$ on $\mathcal{X}$ satisfies the LDP with rate n and with rate function

$$I(z) = \sup_{t\in\mathbb{R}}[zt - \log\varphi(t)], \quad z \in \mathbb{R}. \tag{1.3.3}$$

This result is usually called the level-one LDP. Note that here $\mathcal{X}$ is $\mathbb{R}$. For the case ρ is the standard Gaussian the rate function becomes

$$I(z) = \frac{z^2}{2}, \quad z \in \mathbb{R}. \tag{1.3.4}$$

Next we look at the sequence $(P_n)_{n\in\mathbb{N}}$, where P_n is the law of the *empirical distribution*

$$L_n^{(2)} = \frac{1}{n}\sum_{i=1}^{n} \delta_{X_i}, \tag{1.3.5}$$

where δ_x is the point-mass at $x \in \mathbb{R}$. $L_n^{(2)}$ is a random probability measure on $\mathbb{R}$. The large deviation principle in this case is called Sanov's Theorem [48]. This is also called the level-two LDP. Note that $\mathcal{X}$ here is the set of probability measures on $\mathbb{R}$.

Theorem 1.3.4 (Sanov's Theorem). *The sequence $(P_n)_{n\in\mathbb{N}}$, of the law of the empirical distribution satisfies the LDP on $\mathcal{X}$ with rate n and rate function*

$$I_\rho(\nu) = \begin{cases} \int_{\mathbb{R}} \nu(dx)\log\left(\frac{d\nu}{d\rho}(x)\right), & \textit{if } \nu \ll \rho \\ \infty & \textit{otherwise,} \end{cases} \tag{1.3.6}$$

where $\frac{d\nu}{d\rho}(x)$ is the Radon-Nikodym derivative of ν with respect to ρ and $\nu \ll \rho$ means ν is absolutely continuous with respect to ρ.

$I_\rho(\nu)$ is called the *relative entropy* of ν with respect to ρ, usually written as $h(\nu|\rho)$.

Let $X^{(n)} = (X_1, X_2, \cdots, X_n)^{\text{per}}$ be the periodic extension of the vector $(X_1, X_2, \cdots, X_n)$ to an element in $\mathbb{R}^{\mathbb{N}}$. Consider the sequence $(P_n)_{n\in\mathbb{N}}$ of probability measures on $\mathcal{X}$, where P_n is the law of the *empirical measure*

$$L_n^{(3)} = \frac{1}{n}\sum_{i=1}^{n} \delta_{\tau^i X^{(n)}}, \tag{1.3.7}$$

where τ is the left shift operator acting on $\mathbb{R}^{\mathbb{N}}$. In this case $\mathcal{X}$ is the set of probability measures on $\mathbb{R}^{\mathbb{N}}$ invariant under τ. For any element μ of $\mathcal{X}$ the *specific relative entropy* $H(\mu|\rho^{\mathbb{N}})$ of μ w.r.t. $\rho^{\mathbb{N}}$ is defined as

$$H(\mu|\rho^{\mathbb{N}}) = \lim_{N\to\infty} \frac{1}{N} h(\pi_N \mu|\rho^N), \tag{1.3.8}$$

where $\pi_N\mu$ is the projection of μ onto the first N coordinates.

Theorem 1.3.5. *The sequence $(P_n)_{n\in\mathbb{N}}$ of the laws of the empirical measure satisfies the LDP on $\mathcal{X}$ with rate n and rate function*

$$I_\rho^\infty(\mu) = H(\mu|\rho^{\mathbb{N}}). \tag{1.3.9}$$

See [5] Section 6.5.3 for a proof of this theorem. There is an analogous version of Theorem 1.3.5 if the initial sequence X of random variables is replaced by a family of random variables indexed by $\mathbb{Z}^d$. Here we consider a net of probability measures indexed by progressively increasing subsets of $\mathbb{Z}^d$ that exhaust $\mathbb{Z}^d$. This net of subsets must have a surface–volume ratio that tends to zero. This property is called the *van Hove* property. An example of such a net is the net of boxes $\Lambda_n = \{-n, -n+1, \cdots, n-1, n\}^d$. In this case the empirical measure becomes

$$\bar{L}_n^{(3)} = \frac{1}{|\Lambda_n|}\sum_{x\in\Lambda_n} \delta_{\Theta^x X^{(n)}}, \tag{1.3.10}$$

where $|\Lambda_n|$ is the cardinality of Λ_n, Θ^x is the translation of points in $\mathbb{Z}^d$ by x and $X^{(n)}$ is the periodic extension of elements in $\mathbb{R}^{\Lambda_n}$ to points in $\mathbb{R}^{\mathbb{Z}^d}$. With this choice the LDP rate is $|\Lambda_n|$ and $\mathcal{X}$ is the space of all translation invariant probability measures on $\mathbb{R}^{\mathbb{Z}^d}$. Further, P_n is the law of $\bar{L}_n^{(3)}$. The specific relative entropy for μ in $\mathcal{X}$ w.r.t. $\rho^{\mathbb{Z}^d}$ becomes

$$H(\mu|\rho^{\mathbb{Z}^d}) = \lim_{\Lambda\uparrow\mathbb{Z}^d} \frac{1}{|\Lambda|} h(\pi_\Lambda \mu|\rho^\Lambda), \tag{1.3.11}$$

where $\pi_\Lambda\mu$ is the projection of μ onto the coordinates in Λ and the limit is along a net of subsets of $\mathbb{Z}^d$ that has the van Hove property.

Next we review the tilted LDP. Given a sequence (net) of probability measures satisfying the LDP, the tilted LDP allows us to generate a new sequence (net) of probability measures that also satisfies the LDP. This is achieved by tilting the original sequence with exponential weights.

Theorem 1.3.6 (Tilted LDP). *Let $(P_n)_{n\in\mathbb{N}}$ satisfy the LDP on $\mathcal{X}$ with rate n and with rate function I. Let $F : \mathcal{X} \to \mathbb{R}$ be a continuous function that is bounded from above. Define*

$$J_n(S) = \int_S e^{nF(x)} P_n(dx), \quad \text{with} \quad S \in \mathcal{X} \quad \text{Borel.} \tag{1.3.12}$$

Then the sequence $(P_n^F)_{n\in\mathbb{N}}$ of probability measures, defined by

$$P_n^F(S) = \frac{J_n(S)}{J_n(X)}, \quad \text{with} \quad S \in \mathcal{X} \quad \text{Borel,} \tag{1.3.13}$$

satisfies the LDP on $\mathcal{X}$ with rate n and with rate function

$$I^F(x) = \sup_{y\in\mathcal{X}}[F(y) - I(y)] - [F(x) - I(x)]. \tag{1.3.14}$$

See [10] Section II.7 for a proof of this theorem.

1.3.2 Large deviations for stochastic processes

In this subsection we give LDPs for Brownian motion with small variance and Itô diffusion with small variance. These are LDPs for sequences of probability measures living on the space of paths. The standard Brownian motion result is called Schilder's Theorem [49]. This gives an estimate for the probability that a sample path of Brownian motion with small variance will stray far from the mean path. In this section the space $\mathcal{X}$ is the the Banach space C_0 of continuous functions $f : [0, T] \to \mathbb{R}^d$ such that $f(0) = 0$, equipped with the supremum norm.

Theorem 1.3.7 (Schilder's Theorem). *Let B be a standard d-dimensional Brownian motion starting at the origin. Let P denote the law of B, i.e., the classical Wiener measure. For $n \in \mathbb{N}$, let P_n denote the law of the rescaled process $B/\sqrt{n}$. Then, the sequence of probability measures $(P_n)_{n\in\mathbb{N}}$ satisfies the LDP on $\mathcal{X}$ with rate n and rate function $I : C_0 \to \mathbb{R} \cup \{+\infty\}$ given by*

$$I(\omega) = \begin{cases} \frac{1}{2}\int_0^T |\dot{\omega}(t)|^2 dt & \text{if } \omega_t \text{ is absolute continuous} \\ +\infty & \text{otherwise.} \end{cases} \tag{1.3.15}$$

We now present the Freidlin-Wentzell Theorem [22] which extends the Schilder's Theorem to Itô diffusion with small variance.

Theorem 1.3.8 (Freidlin-Wentzell Theorem). *Let B be a standard d-dimensional Brownian motion starting at the origin. For $n \in \mathbb{N}$, let P_n be the law of the solution X^n of the Itô stochastic differential equation*

$$\begin{cases} dX_t^n = b(X_t^n)dt + \frac{1}{\sqrt{n}} dB_t \\ X_0^n = 0, \end{cases} \tag{1.3.16}$$

where the drift vector field $b : \mathbb{R}^d \to \mathbb{R}^d$ is uniformly Lipschitz continuous. Then, the sequence of probability measures $(P_n)_{n\in\mathbb{N}}$ satisfies the LDP on $\mathcal{X}$ with rate n and rate function

$$I(\omega) = \begin{cases} \frac{1}{2}\int_0^T |\dot{\omega}_t - b(\omega_t)|^2 dt & \text{if } \omega \text{ lies in the Sobolev space } H^1([0,T];\mathbb{R}^d) \\ +\infty & \text{otherwise.} \end{cases} \tag{1.3.17}$$

1.3.3 The Feng-Kurtz scheme

In this section we review the Feng-Kurtz scheme [18] (Example 1.5) for studying the large deviation properties for the trajectories of more general Markov processes. We follow closely Appendix A.2 of [12] to explain this scheme as follows.

Consider a sequence of Markov processes $X = (X_n)_{n\in\mathbb{N}}$ with $X_n = \{X_n(t)\}_{t\geq 0}$, living on a common state space (like $\mathbb{R}$, $\mathbb{R}^d$ or a space of probability measures). Suppose that X_n has generator $\mathcal{L}_n$ and in the limit as $n \to \infty$ converges to a process $(x(t))_{t\geq 0}$, which can be either deterministic or stochastic. Then, by the Markov property, if the sequence P_n of the laws of X_n satisfies the LDP, then the rate function takes the form

$$\bar{\mathcal{I}}(\gamma) = \int_0^T L(\gamma_t, \dot{\gamma}_t)\, dt, \tag{1.3.18}$$

where the function $t \mapsto L(\gamma_t, \dot{\gamma}_t)$ is called the 'Lagrangian' and the dot above γ_t means the derivative with respect to time. The Feng-Kurtz scheme provides a procedure to identify the Lagrangian. We outline the scheme in following four steps:

1. Compute the generator of the non-linear semigroup

$$(\mathcal{H}f)(x) = \lim_{n\to\infty} \frac{1}{n}\, e^{-nf(x)} \left(\mathcal{L}_n e^{nf}\right)(x). \tag{1.3.19}$$

2. Look for a function $H(x,p)$ of two variables such that

$$(\mathcal{H}f)(x) = H(x, \nabla f(x)). \tag{1.3.20}$$

   What ∇f means depends on the context: on $\mathbb{R}^d$ it simply is the gradient of f, while on an infinite-dimensional state space it is a functional derivative.

3. The Lagrangian L is obtained as the Legendre transform of H:

$$L(x,\lambda) = \sup_p \left[\langle p, \lambda\rangle - H(x,p)\right]. \tag{1.3.21}$$

   What $\langle\cdot\rangle$ means also depends on the context: on $\mathbb{R}^d$ it simply is the inner product, while in general it is a natural pairing between a space and its dual, such as $\langle f, \mu\rangle = \int f d\mu$.

4. The Lagrangian in (1.3.18) is the function L with $x = \gamma_t$ and $\lambda = \dot{\gamma}_t$.

The Lagrangian $L(x, \dot{x})$ is exactly the Lagrangian in *Lagrangian mechanics*, with x being interpreted as the (generalized) position and $\dot{x}$ as the (generalized) velocity. The function $H(x, p)$ is called the 'Hamiltonian'. It is exactly the Hamiltonian in *Hamiltonian mechanics*, with x being interpreted as the (generalized) position and p as the (generalized) momentum, but is a completely different object than the spin (e.g. Ising) Hamiltonian. For background of Lagrangian and Hamiltonian mechanics, we refer the reader to [25].

All the above LDP results assume the process starts from a fixed point, say the origin. The question now is "Will these results continue to be true if we start from a randomly chosen point?". This question is answered in the affirmative. The only thing that changes is the rate function. In particular, if the sequence of Markov processes $X = (X_n)_{n\in\mathbb{N}}$, with $X_n = \{X_n(t)\}_{t\geq 0}$, start from the sequence of initial distributions $(\mu_n)_{n\in\mathbb{N}}$ that satisfies the LDP with rate n and rate function I. Then the sequence $X = (X_n)_{n\in\mathbb{N}}$ satisfies the LDP with rate n and rate function

$$\mathcal{I}(\gamma) = I(\gamma_0) + \int_0^T L(\gamma_t, \dot{\gamma}_t)\, dt. \tag{1.3.22}$$

For details, see Feng and Kurtz [18].

1.3.4 Uniqueness and non-uniqueness of optimal trajectories

From Lagrangian mechanics the rate functional $\bar{\mathcal{I}}$ (1.3.18) is the *action functional* associated with the Lagrangian L (1.3.21). The natural question that comes to mind is "What are the trajectories that give rise to the least action?". Such trajectories with least action are the solutions of the Lagrange equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_t} = \frac{\partial L}{\partial x_t} \tag{1.3.23}$$

or, equivalently, the Hamilton equations

$$\dot{x}_t = \frac{\partial H}{\partial p_t}, \qquad \dot{p}_t = -\frac{\partial H}{\partial x_t}. \tag{1.3.24}$$

For the action functional $\mathcal{I}$ (1.3.22), the optimal trajectories have to satisfy the *open-start condition*

$$\left[\frac{\partial L(x_t, \dot{x}_t)}{\partial \dot{x}_t}\right]_{t=0} = \left[\frac{\partial I(x_0)}{\partial x_0}\right]_{x_0=a} \tag{1.3.25}$$

in addition to the above Lagrange's equation.

For the applications in this thesis, we want optimal trajectories associated with the rate functional for the path measure for trajectories with random starting points but ending

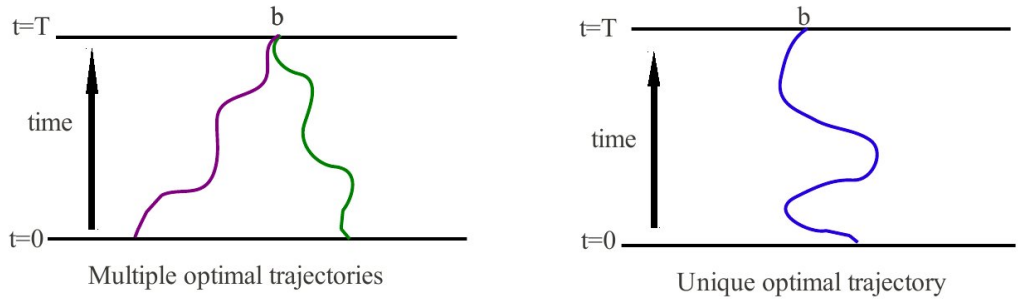

Figure 1.5: Optimal trajectories for path-wise constrained system

at a fixed terminal point. This path measure is what we called the constrained system. The trajectories we consider include trajectories of empirical average (real-valued) (1.3.1), empirical distribution (probability measure on the single-spin space S) (1.3.5) and empirical measure (probability measure on the configuration space Ω) (1.3.7) of configurations of spin systems. The starting configuration of the spin system will be chosen according to a Gibbs measure. The question now is whether the time-evolved measure, on the spin configurations, retains or loses its Gibbs property. The answer to this question is linked to the existence of multiple optimal trajectories for the large deviation rate functional for the constrained system. If there is a unique optimal trajectory connecting any fixed terminal point at time $T > 0$ to a point at time zero then the time-evolved measure at time T is Gibbs. On the other hand, if there are multiple optimal trajectories associated to some fixed terminal point b at time $T > 0$, then the time-evolved measure at time T is non-Gibbs and the terminal point b is said to be bad. This is analogous to the two-layer approach for studying Gibbs-non-Gibbs properties of transforms of Gibbs measures. Uniqueness of optimal trajectory corresponds, in the two-layer picture, to uniqueness of the constrained system. Multiplicity of optimal trajectories corresponds to the occurrence of phase transitions in the constrained system associated to the two-layer approach, see Figure 1.5.

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2

Transformations of one-dimensional Gibbs measures with infinite-range interaction

2.1 Introduction

Local transformations of Gibbs measures can be non-Gibbs. In [1], the mechanism behind the creation of non-Gibbsianness is explained as a hidden phase transition: conditioned on a certain configuration of the transformed spins, the original spins can exhibit a phase transition. Even if the untransformed system is not in a phase transition regime, by conditioning on the transformed configuration we can bring it into a regime of phase transition. In a regime of strong uniqueness, such as the Dobrushin uniqueness regime, or the complete analyticity regime, one expects that Gibbs measures turn into Gibbs measures under stochastic or deterministic disjoint-block transformations.

For one-dimensional systems in the uniqueness regime, one also expects that local transformations conserve the Gibbs property. Using disagreement percolation, this has been proved for finite-range potentials, [9]. The technique of disagreement percolation has however not been extended to the case of infinite range interactions, and in fact (at present) breaks down in that context. Further, it is also known that in the uniqueness regime in dimension one, decimating sufficiently many times brings the system into a regime where cluster expansion can be obtained, and hence the system becomes completely analytic [3]. Finally, in the context of dyamical systems, it has been shown recently [4] that a Gibbs measure with an exponentially decaying interaction transforms into a Gibbs measure with an interaction that decays at least as a stretched exponential under a transformation that

"confuses" symbols (i.e., the transformed spin is determined by a partition of the untransformed spin).

In this paper we consider lattice spin systems in one dimension, with an interaction that is allowed to be of infinite range. We consider single-site stochastic and deterministic transformations. We prove that under a uniqueness condition (see 2.2.8 below), the transformed measure is Gibbs. We further prove that, if the initial interaction is exponentially decaying, then the transformed interaction decays exponentially as well. If the initial interaction decays (in some sense) as a power law with power α (which is chosen big enough to be in the uniqueness regime), then the tranformed interaction can be estimated with a (smaller) power as well.

The method of proof is based on two ingredients. One ingredient is classical: the single-site conditional probabilities of the transformed measure can be written as the expected value of a local function in a Gibbs measure that depends on the conditioning. The dependence on the conditioning, in the case of a single-site transformation is in the form of a spatially varying magnetic field. The second step is to control how the local function expectation depends on this magnetic field. This reduces to the problem of how well a local expectation is approximated by finite-volume Gibbs measure expectations (in a context which is not spatially homogeneous because of the presence of the magnetic field depending on the conditioning). In this second step we use coupling, in the spirit of [2]. As a consequence of this method, we obtain, besides Gibbsianness, estimates on the decay of the transformed potential (where we use the so-called Kozlov potential defined on lattice intervals).

Our paper is organized as follows: we start with basic definitions on Gibbs measures, potentials, and define the transformations that we consider. Section 2.2 is devoted to the case of stochastic single-site transformations. Section 2.3 contains the single-site deterministic case.

2.2 Gibbs measures and their transformations

2.2.1 One-dimensional Gibbs measures

We consider lattice spin systems, with configuration $\Omega = S^{\mathbb{Z}}$, where S, the single-site space, is a finite set. We equip Ω with the product topology. The set of all finite subsets of $\mathbb{Z}$ is denoted by $\mathcal{L}$. For $\Lambda \in \mathcal{L}$ and $\sigma \in \Omega$, we denote by σ_Λ the restriction of σ to Λ, while Ω_Λ denotes the set of all such restrictions.

A function $f : \Omega \to \mathbb{R}$ is called *local* if there exists a finite set $\Delta \subseteq \mathbb{Z}$ such that $f(\eta) = f(\sigma)$ for η and σ coinciding on Δ.

Continuity in the product topology coincides with quasi-locality, i.e., a function $f : \Omega \to \mathbb{R}$ is continuous if and only if it is a uniform limit of local functions, more precisely if

$$\lim_{\Lambda \uparrow \mathbb{Z}} \sup_{\xi,\zeta \in \Omega} |f(\omega_\Lambda \xi_{\Lambda^c}) - f(\omega_\Lambda \zeta_{\Lambda^c})| = 0, \tag{2.2.1}$$

Definition 2.2.1. *A function $\Phi : \mathcal{L} \times \Omega \to \mathbb{R}$ such that $\Phi(A, \sigma)$ depends only on $\sigma(x)$, $x \in A$ for $\forall A \in \mathcal{L}$, is called a **potential**. A potential is **uniformly absolutely convergent** if for all $x \in \mathbb{Z}$*

$$\sum_{A \ni x} \|\Phi(A, \sigma)\|_\infty < \infty, \tag{2.2.2}$$

where $\|\Phi(A, \sigma)\|_\infty = \sup_{\sigma \in \Omega} |\Phi(A, \sigma)|$.

For $\Phi \in \mathcal{B}$, $\zeta \in \Omega$, $\Lambda \in \mathcal{L}$, we define the finite-volume *Hamiltonian* with boundary condition ζ as

$$H_\Lambda^\zeta(\sigma) = \sum_{A \bigcap \Lambda \neq \varnothing} \Phi(A, \sigma_\Lambda \zeta_{\Lambda^c}). \tag{2.2.3}$$

Corresponding to this Hamiltonian we have the *finite-volume Gibbs measures* $\mu_\Lambda^{\Phi,\zeta}$, $\Lambda \in \mathcal{L}$, with boundary condition ζ, defined on Ω by

$$\int f(\xi) \mu_\Lambda^{\Phi,\zeta}(d\xi) = \sum_{\sigma_\Lambda \in \Omega_\Lambda} f(\sigma_\Lambda \zeta_{\Lambda^c}) \frac{\exp\left(-H_\Lambda^\zeta(\sigma)\right)}{Z_\Lambda^\zeta}, \tag{2.2.4}$$

where Z_Λ^ζ denotes the partition function normalizing $\mu_\Lambda^{\Phi,\zeta}$ to a probability measure and $f : \Omega \mapsto \mathbb{R}$ denotes any local function. For a probability measure μ on Ω, we denote by μ_Λ^ζ the condition probability distribution of $\sigma(x)$, $x \in \Lambda$, given $\sigma_{\Lambda^c} = \zeta_{\Lambda^c}$, which is of course only $\mu - a.s.$ defined.

Definition 2.2.2. *For $\Phi \in \mathcal{B}$, we call μ a **Gibbs measure** with potential Φ if a version of its conditional probabilities coincides with the ones prescribed in (2.2.4), i.e., if*

$$\mu_\Lambda^{\Phi,\zeta} = \mu_\Lambda^\zeta \quad \mu - a.s. \quad \forall \Lambda \in \mathcal{L}, \zeta \in \Omega. \tag{2.2.5}$$

We assume that the potential Φ satisfies the following condition.

$$\sup_{i \in \mathbb{Z}} \sum_{A \ni i, diam(A) \geq K} \|\Phi(A, \sigma)\|_\infty = f(K) \tag{2.2.6}$$

where f satisfies

$$\sum_{n=0}^{\infty} f(n) < \infty \tag{2.2.7}$$

Under the condition 2.2.7, the potential Φ admits only one Gibbs measure $\mu = \mu_\Phi$, see [5], section 8.3. Condition 2.2.7 of course implies

$$\lim_{k\to\infty} \sum_{j\geq 0} f(j+k) = 0. \tag{2.2.8}$$

We abbreviate

$$F_k = \sum_{j\geq 0} 2f(j+k) \tag{2.2.9}$$

Remark that in the case of a translation invariant potential, the supremum in (2.2.6) can be omitted and then

$$f(K) = \sum_{A\ni 0, diam(A)\geq K} \|\Phi(A,\sigma)\|_\infty$$

Definition 2.2.3. *A version of conditional probabilities $\{\mu(\cdot|\zeta_{\Lambda^c}) : \zeta_{\Lambda^c} \in \Omega_{\Lambda^c}, \Lambda \in \mathcal{L}\}$ is called **uniformly non null** if for every $\Lambda \in \mathcal{L}$, there exists a constant $m_\Lambda > 0$ such that for every $\omega \in \Omega$*

$$\mu_\Lambda^\omega(\omega) \geq m_\Lambda. \tag{2.2.10}$$

The following theorem due to Kozlov [7] and Sullivan [11] gives a criterion to decide whether a given measure is Gibbsian.

Theorem 2.2.4. *A probability measure μ on $(\Omega, \mathcal{F})$ is a Gibbs measure with respect to a uniformly absolutely convergent potential iff there exists a version of its conditional probabilities that is continuous and uniformly non null.*

Remark 1. *Theorem 2.2.4 is constructive, i.e., the potential is constructed from the conditional probabilities. See section 2.3.1 for the explicit form. In our one-dimensional case, it is non-vanishing on lattice intervals only, i.e., sets of the form $[i,j] = \{i, i+1, \ldots, j\}$. Therefore, if we start from a Gibbs measure we can assume without loss of generality that the potential is non-zero only on lattice intervals.*

2.2.2 Transformations of Gibbs measures

We consider two types of transformation: single-site stochastic tranformations and single-site deterministic transformations.

We first consider single-site stochastic transformation, i.e., for a given σ, the distribution of the image spin configuration is a product measure on $(S')^{\mathbb{Z}}$

$$T(\xi|\sigma) = \prod_{i\in\mathbb{Z}} P_i(\xi_i|\sigma_i). \tag{2.2.12}$$

Here, S' denotes the alphabet of the image-spin, and satisfies $|S'| \leq |S|$.

We assume that the transition kernel of a single site is strictly positive. That is, for $i \in \mathbb{Z}$,

$$\inf_{i\in\mathbb{Z},\xi_i,\sigma_i} P_i(\xi_i|\sigma_i) > 0. \tag{2.2.13}$$

The distribution of the image spin is then defined as

$$\mu \circ T(d\xi) = \int T(d\xi|\sigma)\mu(d\sigma). \tag{2.2.14}$$

The second case is a single-site deterministic transformation $T : \Omega \to \Omega'$ induced by a map $\varphi : S \to S'$ given by

$$(T(\sigma))_i =: \sigma'_i = \varphi(\sigma_i) \tag{2.2.15}$$

2.3 Stochastic single-site transformations

Theorem 2.3.1. *For single site stochastic transformations, if the potential Φ corresponding to the initial Gibbs measure μ satisfies condition (2.2.6), (2.2.7), then the transformed measure $\mu \circ T$ is a Gibbs measure.*

Proof. First of all, $\{\mu \circ T(\cdot|\zeta_{\Lambda^c}) : \zeta_{\Lambda^c} \in \Omega_{\Lambda^c}, \Lambda \in \mathcal{L}\}$ is uniformly non null thanks to the positivity assumption of a single site's transformation kernel in (2.2.13). We then proceed with the proof in two steps.

First, we express the one-site conditional probabilities $\mu \circ T(\xi_0|\xi_{\mathbb{Z}\setminus\{0\}})$ as averages of a local observable over a Gibbs measure depending on the conditioning ξ. This is in the spirit of [8], but simpler since the transformation is stochastic, and hence the "constrained first layer model" of [8] is "not constrained" (given the image configuration, all configurations are possible as originals).

Second, we use a "house-of-cards" coupling technique (see (2.3.7)) in the spirit of [2] to prove the dependence of this local expectation on the conditioning ξ. We restrict to the conditional expectation of the transformed spin at the origin, given the transformed spins outside the origin. The same argument applies to conditional expectation of the spin at any other site.

Step 1.

$$\begin{aligned}
\mu \circ T(\xi_0|\xi_{\mathbb{Z}\setminus\{0\}}) &= \lim_{\Lambda\uparrow\mathbb{Z}} \frac{\mu_\Lambda \circ T(\xi)}{\sum_{\widetilde{\xi}_0} \mu_\Lambda \circ T(\widetilde{\xi}_0\xi_{\Lambda\setminus\{0\}})} \\
&= \lim_{\Lambda\uparrow\mathbb{Z}} \frac{\sum_{\sigma_\Lambda} \mu_\Lambda \circ T(\xi|\sigma_\Lambda)\mu_\Lambda(\sigma_\Lambda)}{\sum_{\sigma_\Lambda}\sum_{\widetilde{\xi}_0} \mu_\Lambda \circ T(\widetilde{\xi}_0\xi_{\Lambda\setminus\{0\}}|\sigma_\Lambda)\mu_\Lambda(\sigma_\Lambda)} \\
&= \lim_{\Lambda\uparrow\mathbb{Z}} \frac{\sum_{\sigma_\Lambda} \prod_i P_i(\xi_i|\sigma_i)\mu_\Lambda(\sigma_\Lambda)}{\sum_{\sigma_\Lambda} \prod_{i\neq 0} P_i(\xi_i|\sigma_i)\mu_\Lambda(\sigma_\Lambda)} \\
&= \lim_{\Lambda\uparrow\mathbb{Z}} \frac{\sum_{\sigma_\Lambda} \prod_i P_i(\xi_i|\sigma_i)\mu_\Lambda(\sigma_\Lambda)}{\sum_{\sigma_\Lambda} \prod_i P_i(\xi_i|\sigma_i)\mu_\Lambda(\sigma_\Lambda)\frac{1}{P_0(\xi_0|\sigma_0)}} \\
&= \left(\mu^\xi\left(\frac{1}{P_0\left(\xi_0|\sigma_0\right)}\right)\right)^{-1} \qquad (2.3.1)
\end{aligned}$$

where μ^ξ is a new Gibbs measure with potential

$$\Phi_A^\xi(\sigma) = \begin{cases} \Phi_A(\sigma) & \text{if } |A| > 1 \\ \Phi_A(\sigma) - \log P_i(\xi_i|\sigma_i) & \text{if } A = \{i\} \end{cases}. \qquad (2.3.2)$$

and where the expectation

$$\left(\mu^\xi\left(\frac{1}{P_0\left(\xi_0|\sigma_0\right)}\right)\right)^{-1}$$

in (2.3.1) is w.r.t. σ_0, with fixed ξ. Remark that this Gibbs measure is uniquely defined, because it is a single-site modification of the original potential Φ, for which we have uniqueness by condition 2.2.8. The equalities in (2.3.1) are almost surely with respect to $\mu \circ T$. Therefore, it suffices to show that $\mu^\xi(P_0^{-1}(\xi_0|\sigma_0))$ is continuous as a function of ξ. Indeed, this then implies that $\mu \circ T(\xi_0|\xi_{\mathbb{Z}\setminus\{0\}})$ admits a version that is continuous as a function of ξ, which implies Gibbsianness, by Theorem 2.2.4. The problem boils down to proving (cf. (2.2.1))

$$\lim_{\Lambda\uparrow\mathbb{Z}} \left|\mu^{\xi_\Lambda\eta_{\Lambda^c}}(P_0^{-1}(\xi_0|\sigma_0)) - \mu^{\xi_\Lambda\eta'_{\Lambda^c}}(P_0^{-1}(\xi_0|\sigma_0))\right| = 0.$$

The form of the potential of $\mu^{\xi_\Lambda\eta_{\Lambda^c}}$, given in (2.3.2), implies that the Hamiltonian of the corresponding finite-volume Gibbs measure $\mu_{\Lambda,\zeta}^{\xi_\Lambda\eta_{\Lambda^c}}$ with boundary condition ζ has the following form

$$H_{\Lambda,\zeta}^{\xi_\Lambda\eta_{\Lambda^c}}(\sigma) = H_{\Lambda,\zeta}(\sigma) - \sum_{i\in\Lambda} \log P_i(\xi_i|\sigma_i).$$

Hence $\mu_{\Lambda,\zeta}^{\xi_\Lambda\eta_{\Lambda^c}}$ is independent of η and denoted as $\mu_{\Lambda,\zeta}^{\xi_\Lambda}$, which implies that

$$\begin{aligned}
&\left|\mu^{\xi_\Lambda\eta_{\Lambda^c}}(P_0^{-1}(\xi_0|\sigma_0)) - \mu^{\xi_\Lambda\eta'_{\Lambda^c}}(P_0^{-1}(\xi_0|\sigma_0))\right| \leq \\
&\left|\mu^{\xi_\Lambda\eta_{\Lambda^c}}(P_0^{-1}(\xi_0|\sigma_0)) - \mu_{\Lambda,\zeta}^{\xi_\Lambda\eta_{\Lambda^c}}(P_0^{-1}(\xi_0|\sigma_0))\right| + \left|\mu_{\Lambda,\zeta}^{\xi_\Lambda\eta'_{\Lambda^c}}(P_0^{-1}(\xi_0|\sigma_0)) - \mu^{\xi_\Lambda\eta'_{\Lambda^c}}(P_0^{-1}(\xi_0|\sigma_0))\right|.
\end{aligned}$$

At this stage, it suffices to prove that, uniformly in ζ,

$$\mu^\xi(P_0^{-1}(\xi_0|\sigma_0)) = \lim_{\Lambda\uparrow\mathbb{Z}} \mu_{\Lambda,\zeta}^{\xi_\Lambda}(P_0^{-1}(\xi_0|\sigma_0)). \qquad (2.3.3)$$

Step 2. It is sufficient for (2.3.3) if we can prove

$$\mu^{\widetilde{\Phi}}(\sigma_0) = \lim_{\Lambda\uparrow\mathbb{Z}} \mu^{\widetilde{\Phi}}_{\Lambda,\zeta}(\sigma_0),$$

where $\widetilde{\Phi}$ is a general potential satisfying condition (2.2.7). More precisely, we will prove that

$$\lim_{l\to\infty} \sup_{\zeta,\zeta'} \left|\mu^{\widetilde{\Phi}}_{[-l,l],\zeta}(\sigma_0) - \mu^{\widetilde{\Phi}}_{[-l,l],\zeta'}(\sigma_0)\right| = 0, \tag{2.3.4}$$

where $\mu^{\widetilde{\Phi}}_{[-l,l],\zeta}$ means the measure for configurations on $[-l,l]$ conditioned on the boundary $\zeta_{[-l,l]^c}$. For simplicity, we will omit the superscript $\widetilde{\Phi}$ hereafter. The speed of this convergence to zero (as a function of l) will determine the decay of the potential associated to the transformed measure (see later).

To prove (2.3.4), we couple the measures $\mu_{[-l,l],\zeta}(\sigma_{[-l,l]} = \cdot)$ and $\mu_{[-l,l],\zeta'}(\sigma_{[-l,l]} = \cdot)$, i.e., we construct a probability measure on pairs $(\sigma^1_{[-l,l]}, \sigma^2_{[-l,l]})$ with marginals $\mu_{[-l,l],\zeta}(\sigma_{[-l,l]} = \cdot)$ and $\mu_{[-l,l],\zeta'}(\sigma_{[-l,l]} = \cdot)$. The construction of the coupling follows an iterative procedure (inspired by [6], Section 7), where we generate in every stage a pair of two spins corresponding to the interior boundary spins at that stage. Initially, we generate $(\sigma^1_{-l}, \sigma^1_l)$ and $(\sigma^2_{-l}, \sigma^2_l)$ according to the maximal coupling[1] of $\mu_{[-l,l],\zeta}(\sigma_{-l} = \cdot, \sigma_l = \cdot)$ and $\mu_{[-l,l],\zeta'}(\sigma_{-l} = \cdot, \sigma_l = \cdot)$. Having generated $(\sigma^i_{-l}, \sigma^i_l)$,$(\sigma^i_{-l+1}, \sigma^i_{l-1})$ ... $(\sigma^i_{-l+m}, \sigma^i_{l-m})$, for $i = 1, 2$, we generate $(\sigma^1_{-l+m+1}, \sigma^1_{l-m-1})$ and $(\sigma^2_{-l+m+1}, \sigma^2_{l-m-1})$ according to the maximal coupling of

$$\mu_{[-l+m+1,l-m-1],\zeta\sigma^1_{[-l+1,-l+m]\bigcup[l-1,l-m]}}(\sigma_{-l+m+1} = \cdot, \sigma_{l-m-1} = \cdot)$$

and

$$\mu_{[-l+m+1,l-m-1],\zeta'\sigma^2_{[-l+1,-l+m]\bigcup[l-1,l-m]}}(\sigma_{-l+m+1} = \cdot, \sigma_{l-m-1} = \cdot).$$

To estimate $|\mu_{[-l,l],\zeta}(\sigma_0) - \mu_{[-l,l],\zeta'}(\sigma_0)|$, we use the coupling just described, and proceed as in a "house-of-cards coupling" method of Bressaud-Fernández-Galves [2]. When we generate the symbols $\sigma_{-l+k}, \sigma_{l-k}$, we think of this as being at time instant k in the coupling. Suppose that for the last m time instants in the coupling, we had matches, then as in [2] we have to estimate the probability of a mismatch at time instant $m+1$. This is done in the next lemma.

Lemma 2.3.2. *For $-l < -n_2 < -n_1 \le 0 \le n_1 < n_2 < l$, $n_2 - n_1 = m$, let ξ and ζ be two configurations on the complement of $[-n_1, n_1]$ such that they agree on $\Delta_m = [-n_2, -n_1 - 1]\bigcup[n_1 + 1, n_2]$, then*

$$\sup_{\alpha,\beta,\zeta,\xi,\zeta_{\Delta_m}=\xi_{\Delta_m}} |\mu_{[-n_1,n_1],\zeta}(\sigma_{-n_1} = \alpha, \sigma_{n_1} = \beta) - \mu_{[-n_1,n_1],\xi}(\sigma_{-n_1} = \alpha, \sigma_{n_1} = \beta)| \le 2(e^{F_m} - 1),$$

where F_m is defined in (2.2.9).

[1] For details of coupling and maximal coupling, we refer to [12].

Proof. Start with

$$\mu_{[-n_1,n_1],\zeta}(\sigma_{-n_1}=\alpha,\sigma_{n_1}=\beta)=\sum_{\sigma'}\frac{e^{-H^{\zeta}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}{Z^{\zeta}_{[-n_1,n_1]}},$$

where we abbreviated $\alpha\sigma'\beta$ to be the configuration $\sigma_{[-n_1,n_1]}$ with $\sigma_{-n_1}=\alpha$, $\sigma_{n_1}=\beta$ and $\sigma_{[-n_1+1,n_1-1]}=\sigma'$, and where the sum runs over all configurations σ' on $[-n_1+1,n_1-1]$. We then proceed as follows:

$$\begin{aligned}
&\sup_{\alpha\sigma'\beta,\zeta,\xi,\zeta_{\Delta_m}=\xi_{\Delta_m}}\left|\mu_{[-n_1,n_1],\zeta}(\sigma_{-n_1}=\alpha,\sigma_{n_1}=\beta)-\mu_{[-n_1,n_1],\xi}(\sigma_{-n_1}=\alpha,\sigma_{n_1}=\beta)\right|\\
&=\sup_{\alpha\sigma'\beta,\zeta,\xi,\zeta_{\Delta_m}=\xi_{\Delta_m}}\left|\sum_{\sigma'}\frac{e^{-H^{\zeta}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}{Z^{\zeta}_{[-n_1,n_1]}}-\sum_{\sigma'}\frac{e^{-H^{\xi}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}{Z^{\xi}_{[-n_1,n_1]}}\right|\\
&\le\sup_{\alpha\sigma'\beta,\zeta,\xi,\zeta_{\Delta_m}=\xi_{\Delta_m}}\left\{\left|\frac{\sum_{\sigma'}e^{-H^{\zeta}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}{Z^{\zeta}_{[-n_1,n_1]}}-\frac{\sum_{\sigma'}e^{-H^{\xi}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}{Z^{\zeta}_{[-n_1,n_1]}}\right|\right.\\
&\qquad\left.+\left|\frac{\sum_{\sigma'}e^{-H^{\xi}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}{Z^{\zeta}_{[-n_1,n_1]}}-\frac{\sum_{\sigma'}e^{-H^{\xi}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}{Z^{\xi}_{[-n_1,n_1]}}\right|\right\}\\
&\le\sup_{\alpha\sigma'\beta,\zeta,\xi,\zeta_{\Delta_m}=\xi_{\Delta_m}}\left\{\left|\frac{\sum_{\sigma'}e^{-H^{\zeta}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}{\sum_{\sigma'}e^{-H^{\xi}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}-1\right|+\left|\frac{Z^{\xi}_{[-n_1,n_1]}}{Z^{\zeta}_{[-n_1,n_1]}}-1\right|\right\}\\
&=\sup_{\alpha\sigma'\beta,\zeta,\xi,\zeta_{\Delta_m}=\xi_{\Delta_m}}\left\{\left|\frac{\sum_{\sigma'}e^{-H^{\zeta}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}{\sum_{\sigma'}e^{-H^{\xi}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}-1\right|+\left|\frac{\sum_{\alpha'\sigma'\beta'}e^{-H^{\zeta}_{[-n_1,n_1]}(\alpha'\sigma'\beta')}}{\sum_{\alpha'\sigma'\beta'}e^{-H^{\xi}_{[-n_1,n_1]}(\alpha'\sigma'\beta')}}-1\right|\right\},
\end{aligned}$$

where the sums in the second fraction run over all configuration $\alpha'\sigma'\beta'$ on $[-n_1,n_1]$. By using the elementary inequalities $\min_{i\in\{1,\dots,n\}}\frac{a_i}{b_i}\le\frac{\sum_{i=1}^n a_i}{\sum_{i=1}^n b_i}\le\max_{i\in\{1,\dots,n\}}\frac{a_i}{b_i}$ and $|e^x-1|\le e^{|x|}-1$, we obtain

$$\begin{aligned}
&\sup_{\alpha\sigma'\beta,\zeta,\xi,\zeta_{\Delta_m}=\xi_{\Delta_m}}\left\{\left|\frac{\sum_{\sigma'}e^{-H^{\zeta}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}{\sum_{\sigma'}e^{-H^{\xi}_{[-n_1,n_1]}(\alpha\sigma'\beta)}}-1\right|+\left|\frac{\sum_{\alpha'\sigma'\beta'}e^{-H^{\zeta}_{[-n_1,n_1]}(\alpha'\sigma'\beta')}}{\sum_{\alpha'\sigma'\beta'}e^{-H^{\xi}_{[-n_1,n_1]}(\alpha'\sigma'\beta')}}-1\right|\right\}\\
&\le\sup_{\alpha\sigma'\beta,\zeta,\xi,\zeta_{\Delta_m}=\xi_{\Delta_m}}\left\{\left(e^{\sup_{\sigma'}\left|H^{\xi}_{[-n_1,n_1]}(\alpha\sigma'\beta)-H^{\zeta}_{[-n_1,n_1]}(\alpha\sigma'\beta)\right|}-1\right)\right.\\
&\qquad\left.+\left(e^{\sup_{\alpha'\sigma'\beta'}\left|H^{\xi}_{[-n_1,n_1]}(\alpha'\sigma'\beta')-H^{\zeta}_{[-n_1,n_1]}(\alpha'\sigma'\beta')\right|}-1\right)\right\}\\
&=2\left(e^{\sup_{\zeta,\xi,\zeta_{\Delta_m}=\xi_{\Delta_m},\alpha\sigma'\beta}\left|H^{\xi}_{[-n_1,n_1]}(\alpha\sigma'\beta)-H^{\zeta}_{[-n_1,n_1]}(\alpha\sigma'\beta)\right|}-1\right),
\end{aligned}$$

Now

$$\begin{aligned}
&\sup_{\alpha\sigma'\beta,\zeta,\xi,\zeta_{\Delta_m}=\xi_{\Delta_m}} \left| H^{\xi}_{[-n_1,n_1]}(\alpha\sigma'\beta) - H^{\zeta}_{[-n_1,n_1]}(\alpha\sigma'\beta) \right| \\
\leq & \sum_{j=-n_1}^{n_1} \sum_{A\ni j, diam(A)\geq (n_2-j)\bigwedge(j-(-n_2))} 2 \parallel \Phi(A,\sigma) \parallel_\infty \\
\leq & \sum_{k=0}^{2n_1} \sup_{j\in\mathbb{Z}} \sum_{A\ni j, diam(A)\geq k+m} 2 \parallel \Phi(A,\sigma) \parallel_\infty \\
\leq & \sum_{k=0}^{\infty} 2f(k+m) = F_m.
\end{aligned}$$

(Recall for the above inequalities that $m = n_2 - n_1$.) □

As a consequence of the lemma, the probability of mismatch after m matches is dominated by

$$\gamma_m := 2(e^{F_m} - 1), \tag{2.3.5}$$

Then the probability that we are not coupled at time $k = l$ (i.e., the spins at the origin in the coupling are unequal) can be estimated by

$$\left|\mu_{[-l,l],\zeta}(\sigma_0) - \mu_{[-l,l],\zeta'}(\sigma_0)\right| = \left|\mathbb{E}_{\mathbb{P}_{12}}(\sigma_0^1 - \sigma_0^2)\right|$$

where $\mathbb{P}_{12}$ denotes the coupling of the measures $\mu_{[-l,l],\zeta}(\sigma_{[-l,l]} = \cdot)$ and $\mu_{[-l,l],\zeta'}(\sigma_{[-l,l]} = \cdot)$ just described.

Remark that by the non-nulness of Gibbs measures, we have that

$$\sup_{\alpha,\beta,\zeta,\xi,\zeta_{\Delta_m}=\xi_{\Delta_m}} \mu_{[-n_1,n_1],\zeta}(\sigma_{-n_1} = \alpha, \sigma_{n_1} = \beta) < 1 - \delta$$

for some $0 < \delta < 1$. As in [2], we then consider the auxiliary Markov chain S_n on $\{0, 1, 2, \cdots\}$ whose transition probabilities are

$$\begin{cases} \mathbb{P}(S_{n+1} = m+1 | S_n = m) = 1 - \min\{\gamma_m, 1-\delta\} \\ \mathbb{P}(S_{n+1} = 0 | S_n = m) = \min\{\gamma_m, 1-\delta\}. \end{cases} \tag{2.3.6}$$

On the other hand, we have the process that counts the number of matches (the so-called "house-of-cards" process), defined by

$$\begin{cases} Z_0 = 0 \\ Z_{n+1} = \begin{cases} Z_n + 1 & \text{if } (\sigma^1_{-l+n}, \sigma^1_{l-n}) = (\sigma^2_{-l+n}, \sigma^2_{l-n}) \\ 0 & \text{otherwise} \end{cases} \quad \text{for } n = 0, 1, 2, \ldots \end{cases} \tag{2.3.7}$$

By Proposition 1 in [2], we have

$$\left|\mu_{[-l,l],\zeta}(\sigma_0) - \mu_{[-l,l],\zeta'}(\sigma_0)\right| = \left|\mathbb{E}_{\mathbb{P}_{12}}(\sigma_0^1 - \sigma_0^2)\right| = \mathbb{P}(Z_l = 0) \leq \mathbb{P}(S_l = 0). \tag{2.3.8}$$

Finally condition (2.2.8) insures that $\gamma_n \to 0$ as $n \to +\infty$. Then by Proposition 2 in [2], we have $\mathbb{P}(S_l = 0) \to 0$ as $l \to +\infty$, which completes the proof. □

2.3.1 The transformed potential

Definition 2.3.3. *If μ is a measure that admits a continuous version of the conditional probabilities $\mu(\xi_i|\xi_{\mathbb{Z}\setminus\{i\}})$, $i \in \mathbb{Z}$, then we call φ an estimate for the rate of continuity if*

$$\sup_{\xi,\zeta} \left|\mu(\xi_i|\xi_{[-n,n]\setminus\{i\}}\zeta_{[-n,n]^C}) - \mu(\xi_i|\xi_{\mathbb{Z}\setminus\{i\}})\right| \leq \varphi(n). \tag{2.3.9}$$

In the previous section we showed that for our transformed Gibbs measure, $\mathbb{P}(S_n = 0)$ is an estimate for the rate of continuity. We now show the decay of the Kozlov potential associated to μ, when we have an estimate on the rate of continuity. We start from the following explicit form of the potential of theorem 2.2.4, see [7], [10]. We assume, without loss of generality, that the finite alphabet contains a distinguished symbol denoted by "$+$".

Theorem 2.3.4. *Let ν be a probability measure such that the conditional probabilities $\nu(\xi_i|\xi_{\mathbb{Z}\setminus\{i\}})$, $i \in \mathbb{Z}$, are non null and have a continuous version. Consider the potential, defined on lattice intervals (and vanishing on other subsets) by*

$$U([i,j],\xi) = \log \frac{\nu(\xi_i|\xi_{]i,j[}+)\nu(\xi_j|\xi_{]i,j[}+)}{\nu(\xi_i\xi_j|\xi_{]i,j[}+)}, \tag{2.3.10}$$

where the plus signs mean that conditioned sites outside the lattice interval $[i,j]$ all have the state $+$. If U is uniformly absolutely convergent, then ν is a Gibbs measure associated with the potential U.

We look now at this potential in our context, i.e., when ν is the transformed Gibbs measure $\mu \circ T$. By Theorem 2.3.1, $\mathbb{P}(S_n = 0)$ is an estimate for the rate of continuity of $\mu \circ T$. We can then estimate the potential: if φ is an estimate for the rate of continuity,

$$\begin{aligned} \nu(\xi_i|\xi_{]i,j[}+) &= \nu(\xi_i|\xi_{]i,j]}+)\nu(\xi_j|\xi_{]i,j[}+) + \sum_{\eta_j \neq \xi_j} \nu(\xi_i|\xi_{]i,j[}\eta_j+)\nu(\eta_j|\xi_{]i,j[}+) \\ &\leq \nu(\xi_i|\xi_{]i,j]}+)\left(1 + C\varphi(|j-i|)\right), \end{aligned} \tag{2.3.11}$$

where the constant C is bounded by the non-nullness assumption. Further, we have

$$\nu(\xi_i\xi_j|\xi_{]i,j[}+) = \nu(\xi_i|\xi_{]i,j]}+)\nu(\xi_j|\xi_{[i,j[}+).$$

So we have the estimate on Kozlov potential of the transformed measure

$$\left|U_{[i,j]}(\xi)\right| \leq \log(1 + C\varphi(|j-i|)) \leq C\varphi(|j-i|) \tag{2.3.12}$$

We now consider two relevant cases, according to behavior of F_m in (2.2.9).

1. If f in (2.2.6) decays *exponentially*, then F_N decays also exponentially as N increases. This implies that φ in (2.3.12) also decays exponentially, that is,

$$U_{[i,j]}(\xi) \leq e^{-\lambda|j-i|} \tag{2.3.13}$$

for some $\lambda > 0$.

2. In case that f decays as *a power law* i.e., for some $C > 0$,

$$f(k) \leq \frac{C}{k^\alpha}, \quad \text{for } \alpha > 1, \tag{2.3.14}$$

we have

$$F_N \leq \frac{C_1}{N^{\alpha-1}}, \tag{2.3.15}$$

where C_1 is a positive constant. This implies that φ in (2.3.9) decays as $\frac{C_1}{n^{\alpha-1}}$, which in turn implies that the transformed potential decays as

$$\|U_{[i,j]}\|_\infty \leq \frac{C_1}{(j-i)^{\alpha-1}}. \tag{2.3.16}$$

Hence, $\alpha > 2$ is sufficient to have uniform absolute summability of this potential (whereas $\alpha > 1$ is sufficient for Gibbsianness of the transformed measure)

E.g., if the original potential is a long-range Ising potential, i.e.,

$$\Phi(\{i,j\},\sigma) = \frac{\sigma_i\sigma_j}{|j-i|^\gamma}$$

then we need $\gamma > 2$ for the transformed measure to be Gibbsian, and $\gamma > 3$ for the transformed potential to be uniformly absolute convergent. Remark that for $\gamma < 2$ we do not have uniqueness of the associated Gibbs measure, so the transformed measure might be non-Gibbsian.

2.4 Deterministic single-site transformations

As before, we consider the configuration space of the untransformed system $\Omega = S^{\mathbb{Z}}$, where S is a finite set, and the configuration space of the transformed system is $\Omega' = (S')^{\mathbb{Z}}$. The transformation $T : \Omega \to \Omega'$ now is induced by a map $\varphi : S \to S'$, via

$$(T(\sigma))_i =: \sigma'_i = \varphi(\sigma_i) \tag{2.4.1}$$

This is equivalent with defining the new spin σ_i via a partition of the single-site space S, which in the case of $S = \{1, \ldots, q\}$ and Φ the potential of the Potts-model has been called the fuzzy Potts model, see [9].

To deal with such transformations, we follow the approach of in [8]. This consists of writing the single-site conditional probabilities of the transformed measure in terms of a so-called *constrained restricted first layer measure*. The difference with stochastic transformations is that this measure does not necessarily have full support, i.e., given the second layer constraint $\xi \in \Omega'$, the first layer has to be such that its image coincides with ξ'.

As in the previous section, we start with a Gibbs measure μ on configurations $\sigma \in \Omega$. The potential Φ satisfies (2.2.8). We further abbreviate $\nu = \mu \circ T$ and $K(\eta_i|\sigma_i) = I(\varphi(\sigma_i) = \eta_i)$, where I denotes indicator, and for $\Lambda \subseteq \mathbb{Z}$ finite, $\Lambda_0 := \Lambda \setminus \{0\}$.

For clarity, we first repeat the main steps of [8] to rewrite the single-site conditional probabilities of ν in terms of a constrained restricted first layer measure.

$$\begin{aligned} \nu(\eta_0|\eta_{\Lambda_0}) &= \frac{\sum_{\sigma_\Lambda} \mu(\sigma_\Lambda) \prod_{i\in\Lambda} K(\eta_i|\sigma_i)}{\sum_{\sigma_\Lambda} \mu(\sigma_\Lambda) \prod_{i\in\Lambda_0} K(\eta_i|\sigma_i)} \\ &= \frac{\int \mu(d\zeta) \sum_{\sigma_\Lambda} \mu_{\Lambda,\zeta}(\sigma_\Lambda) \prod_{i\in\Lambda} K(\eta_i|\sigma_i)}{\int \mu(d\zeta) \sum_{\sigma_\Lambda} \mu_{\Lambda,\zeta}(\sigma_\Lambda) \prod_{i\in\Lambda_0} K(\eta_i|\sigma_i)} \end{aligned} \tag{2.4.2}$$

Now we consider the following auxiliary measure on the state space $\Omega_0 := S^{\Lambda_0}$.

$$\mu^{\eta_{\Lambda_0}}_{\Lambda_0,\zeta}(\sigma_{\Lambda_0}) := \frac{1}{N^\eta_{\Lambda,\zeta}} \exp\left(-\mathcal{H}^\zeta_{\Lambda_0}(\sigma_{\Lambda_0})\right) \prod_{i\in\Lambda_0} K(\eta_i|\sigma_i) \tag{2.4.3}$$

where $N^\eta_{\Lambda,\zeta}$ denotes the normalizing constant, and

$$\mathcal{H}^\zeta_{\Lambda_0}(\sigma_{\Lambda_0}) = \sum_{A\cap\Lambda_0\neq\varnothing, A\not\ni 0} \Phi(A, \sigma_\Lambda \zeta_{\Lambda^c}) \tag{2.4.4}$$

These measures concentrate on configurations $\sigma_{\Lambda_0} \in S^{\Lambda_0}$ compatible with η_{Λ_0}, i.e., such that $K(\eta_i|\sigma_i) \neq 0$ for all $i \in \Lambda_0$. For $\eta \in \Omega'$ fixed, they form a η-dependent specification on the configuration space $S^{\mathbb{Z}_0}$, i.e.,

a) $\mu^{\eta_{\Lambda_0}}_{\Lambda_0,\zeta}(\sigma_{\Lambda_0})$ is a probability measure on S^{Λ_0}

b) $\mu^{\eta_{\Lambda_0}}_{\Lambda_0,\zeta}(\sigma_{\Lambda_0})$ depends only in ζ on $\mathbb{Z}_0 \setminus \Lambda_0$

c) Consistency: if we denote

$$\left(\gamma^\eta_{\Lambda_0}(g)\right)(\zeta) := \int \mu^{\eta_{\Lambda_0}}_{\Lambda_0,\zeta}(d\sigma_{\Lambda_0}) g(\sigma_{\Lambda_0}\zeta_{\Lambda^c}) \tag{2.4.5}$$

then these η-dependent kernels γ^η_Λ satisfy

$$\gamma^\eta_{\Lambda_0}(\gamma^\eta_{\Lambda'_0}(g)) = \gamma^\eta_{\Lambda_0}(g) \tag{2.4.6}$$

for all $\Lambda \supset \Lambda'$ and all local functions g.

In terms of these measures, we can rewrite the conditional probability $\nu(\eta_0|\eta_{\Lambda_0})$ as follows.

$$\nu(\eta_0|\eta_{\Lambda_0}) = \frac{\int \mu(d\zeta) \frac{N^\eta_{\Lambda,\zeta}}{Z^\zeta_\Lambda} \int \mu^{\eta_{\Lambda_0}}_{\Lambda_0,\zeta}(d\sigma_{\Lambda_0}) \psi^\zeta_{0,\Lambda}(\eta_0, \sigma_{\Lambda_0})}{\int \mu(d\zeta) \frac{N^\eta_{\Lambda,\zeta}}{Z^\zeta_\Lambda} \int \mu^{\eta_{\Lambda_0}}_{\Lambda_0,\zeta}(d\sigma_{\Lambda_0}) \varphi^\zeta_{0,\Lambda}(\sigma_{\Lambda_0})} \tag{2.4.7}$$

where

$$\begin{aligned} \psi^\zeta_{0,\Lambda}(\eta_0, \sigma_{\Lambda_0}) &= \sum_{\sigma_0} e^{-h_0(\sigma_0 \sigma_{\Lambda_0} \zeta_{\Lambda^c})} K(\eta_0|\sigma_0) \\ \varphi^\zeta_{0,\Lambda}(\sigma_{\Lambda_0}) &= \sum_{\sigma_0} e^{-h_0(\sigma_0 \sigma_{\Lambda_0})\zeta_{\Lambda^c})} \end{aligned} \tag{2.4.8}$$

with

$$h_0(\sigma) = \sum_{A \ni 0} \Phi(A, \sigma) \tag{2.4.9}$$

and Z^ζ_Λ is the finite-volume partition function with boundary condition ζ, i.e.,

$$Z^\zeta_\Lambda = \sum_{\sigma_\Lambda} e^{-H^\zeta_\Lambda(\sigma_\Lambda)}$$

Notice that $\psi^\zeta_{0,\Lambda}(\eta_0, \sigma_{\Lambda_0})$ and $\varphi^\zeta_{0,\Lambda}(\sigma_{\Lambda_0})$ converge uniformly (in η_0, σ, ζ), as $\Lambda \uparrow \mathbb{Z}$ to

$$\begin{aligned} \psi_0(\eta_0, \sigma_{\mathbb{Z}\setminus\{0\}}) &= \sum_{\sigma_0} e^{-h_0(\sigma)} K(\eta_0|\sigma_0) \\ \varphi_0(\sigma_{\mathbb{Z}\setminus\{0\}}) &= \sum_{\sigma_0} e^{-h_0(\sigma)} \end{aligned} \tag{2.4.10}$$

2.4.1 Exponentially decaying potential

Let us now first look at the case where Φ decays exponentially. As a consequence, the decay to zero in (2.2.8) is exponential in k. We will prove here, that, as in the stochastic case, the transformed measure ν has an exponentially decaying interaction as well. In this case, for $\Lambda = [-n, n]$ there exist $C_1, c_1 > 0$ such that for all ζ, σ, η,

$$|\psi^\zeta_{0,\Lambda}(\eta_0, \sigma_{\Lambda_0}) - \psi_0(\eta_0, \sigma_{\mathbb{Z}\setminus\{0\}})| \leq C_1 e^{-c_1 n}$$

and similarly for φ_0. Our aim is then to show that there exist $C_2, c_2 > 0$ such that for all η, $n, m > n$,

$$|\nu(\eta_0|\eta_{[-n,n]_0}) - \nu(\eta_0|\eta_{[-m.m]_0})| \leq C_2 e^{-c_2 n}$$

The idea is once more to couple the measures $\mu^{\eta_{\Lambda_0}}_{\Lambda,\zeta}$ and $\mu^{\eta_{\Lambda_0}}_{\Lambda,\zeta'}$ for different boundary conditions, such that in the coupling the probability that $\sigma^1_i \neq \sigma^2_i$ is bounded by $e^{-\alpha|n-i|\wedge|-n-i|}$ for some $\alpha > 0$. This coupling follows the same iterative procedure as in the stochastic

case, and the estimates are identical. Next, we need to compare expectations of the functions ψ_0, φ_0 (instead of a function that only depends on σ_0 in the stochastic case). These functions ψ_0, φ_0 can however be exponentially well approximated by local functions. We spell out these steps in three lemmas.

Lemma 2.4.1. *Let μ_1, μ_2 be two probability measures on S^{Λ_0} and $\mathbb{P}$ a coupling of them. Then for all functions $g : S^{\Lambda_0} \to \mathbb{R}$ we have*

$$\left| \int g \, d\mu_1 - \int g \, d\mu_2 \right| \leq \sum_{i \in \Lambda_0} \mathbb{P}(\sigma_i^1 \neq \sigma_i^2) \delta_i g \tag{2.4.11}$$

where $\delta_i g(\sigma) = \sup\{g(\sigma) - g(\sigma') : \sigma_j = \sigma'_j \ \forall \ j \neq i\}$

Proof. This is elementary and left to the reader. □

Lemma 2.4.2. *For $\Lambda = [-n, n]$ there exists a coupling $\mathbb{P}$ of $\mu_{\Lambda,\zeta}^{\eta_{\Lambda_0}}$ and $\mu_{\Lambda,\zeta'}^{\eta_{\Lambda_0}}$ such that*

$$\mathbb{P}(\sigma_i^1 \neq \sigma_i^2) \leq C_3 e^{-c_3 |n-i| \wedge |-n-i|} \tag{2.4.12}$$

where $C_3, c_3 > 0$ do not depend on ζ, ζ', n.

Proof. The coupling follows the iterative procedure as in the stochastic case, and the estimates in terms of the function f in (2.2.6) are identical. □

As a consequence of these lemmas we have the existence of a unique Gibbs measure μ^η on $S^{\mathbb{Z}_0}$ consistent with the specification $\mu_{\Lambda,\zeta}^{\eta_{\Lambda_0}}$, and for any local function g (with dependence set in Λ) we have the estimate

$$\sup_\xi \left| \int g d\mu^\eta - \gamma_\Lambda^\eta(\xi)(g) \right| \leq C_3 \sum_i \delta_i(g) e^{-c_3 |n-i| \wedge |-n-i|} \tag{2.4.13}$$

where we used the notation (2.4.5) and where $\Lambda = [-n, n]$

Lemma 2.4.3. *Suppose that $g : S^{\mathbb{Z}_0} \to \mathbb{R}$ is continuous and such that there exist g_k depending only on $\sigma_i, i \in [-k, k]_0$ such that*

$$\|g_k - g\|_\infty < C_4 e^{-c_4 k} \tag{2.4.14}$$

for some $C_4, c_4 > 0$. Then there exists $C_5, c_5 > 0$ such that for $\Lambda = [-n, n]$

$$\sup_\eta \left| \gamma_\Lambda^\eta(g) - \int g \, d\mu^\eta \right| \leq C_5 e^{-c_5 n} \tag{2.4.15}$$

Proof. Choose $\Lambda = [-n, n]$, and choose g_k as in (2.4.14). Write

$$|\gamma_\Lambda^\eta(g)(\zeta) - \gamma_\Lambda^\eta(g)(\xi)| \leq A + B + C \tag{2.4.16}$$

where

$$A := |\gamma_\Lambda^\eta(g)(\zeta) - \gamma_\Lambda^\eta(g_k)(\zeta)| \leq \|g - g_k\|_\infty \tag{2.4.17}$$

$$C := |\gamma_\Lambda^\eta(g_k)(\xi) - \gamma_\Lambda^\eta(g)(\xi)| \leq \|g - g_k\|_\infty \tag{2.4.18}$$

$$B := |\gamma_\Lambda^\eta(g_k)(\zeta) - \gamma_\Lambda^\eta(g_k)(\xi)| \leq 2 \sup_\xi \left| \gamma_\Lambda^\eta(g_k)(\xi) - \int g_k d\mu^\eta \right| \tag{2.4.19}$$

Now use (2.4.13), and the obvious inequality $\delta_i(g) \leq 2\|g\|_\infty$ to obtain

$$|\gamma_\Lambda^\eta(g)(\zeta) - \gamma_\Lambda^\eta(g)(\xi)| \leq 2C_4 e^{-c_4 k} + 4 \sup_k \|g_k\|_\infty \sum_{j=0}^{k} C_3 e^{-c_3(n-j)} \tag{2.4.20}$$

Finally, choose $k = n/2$. □

2.4.2 Power-law decaying potential

For the case where Φ decays according to a power law, more precisely, if

$$f(K) \leq Ck^{-\alpha} \tag{2.4.21}$$

where f is the function associated to the potential Φ as in (2.2.6), and $\alpha > 2$. Then we have the analogue of (2.4.12) (cf. the two cases considered after Theorem 2.3.4)

$$\mathbb{P}(\sigma_i^1 \neq \sigma_i^2) \leq C_3 \left((n - i) \wedge (-n - i)\right)^{\alpha - 1} \tag{2.4.22}$$

Next, the local approximations of the functions ψ_0 and φ_0 converge now only at power-law speed, i.e., the local approximations ψ_0^k, φ_0^k with dependence set $[-k, k]$ satisfy

$$\|\psi_0 - \psi_0^k\|_\infty < Ck^{-\alpha}, \ \|\varphi_0 - \varphi_0^k\|_\infty < Ck^{-\alpha}$$

Therefore, in that case we find, using the same steps as in the exponential case, for all η, $n, m > n$,

$$|\nu(\eta_0|\eta_{[-n,n]_0}) - \nu(\eta_0|\eta_{[-m.m]_0})| \leq C_2 n^{-(\alpha-2)}$$

2.5 Finite-block transformations

We consider finite-block transformations, i.e., in the stochastic case the transition kernel is given by

$$T(\xi|\sigma) = \prod_{i\in\mathbb{Z}} P_i(\xi_i|\sigma_{B_i}) \tag{2.5.1}$$

and in the deterministic case is given by

$$K(\eta_i|\sigma_{B_i}) = I(\varphi(\sigma_{B_i}) = \eta_i) \tag{2.5.2}$$

with $B_i \in \mathcal{L}$ for all $x \in \mathbb{Z}$. We assume again that the transition kernel is strictly positive. Then all the results obtained in the single-site transformation case are still valid if the transformation is stochastic and are still valid in the case of deterministic transformations if $B_i \in \mathcal{L}$, for all $x \in \mathbb{Z}$, are disjoint with each other.

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3

Gibbs-non-Gibbs transitions via large deviations: computable examples

3.1 Introduction

Starting from [3] dynamical Gibbs-non-Gibbs transitions have been considered by several authors, see e.g. [2], [12], [6]. In these studies, one considers lattice spin systems started from a Gibbs measure μ at time zero and evolves it according to a Markovian dynamics (e.g. Glauber dynamics) with stationary Gibbs measure $\nu \neq \mu$. The question is then whether μ_t, the time-evolved measure at time $t > 0$ is a Gibbs measure. Typically this is the case for short times, whereas for longer times, there can be transitions from Gibbs to non-Gibbs (loss) and back from non-Gibbs to Gibbs (recovery). The notion of a "bad configuration", i.e., a point of essential discontinuity of the conditional probabilities of the measure μ_t is crucial here. Such a configuration η_{spec} is typically identified by looking at the joint distribution of the system at time 0 and at time t. If conditioned on η_{spec} the system at time zero has a phase transition, then typically η_{spec} is a bad configuration.

In the context of mean-field models, the authors in [10] started with an analysis of the most probable trajectories (in the sense of large deviations) of a system conditioned to arrive at time T at a given configuration. The setting of [10] is the Curie-Weiss model subjected to a spin-flip dynamics. A Gibbs-non-Gibbs transition is in this context rephrased as a phenomenon of "competing histories", i.e., for special terminal conditions x_{spec} and times T not too small, multiple trajectories can minimize the rate function, and these trajectories can be selected by suitably approximating x_{spec}. Multiple histories were then shown to lead to jumps in conditional probabilities indicating non-Gibbsian behavior in the mean-field

setting, see e.g. [5],[9],[11]. These special conditionings leading to multiple histories are the analogue of "bad configurations" (essential points of discontinuity of conditional probabilities of the measure at time t) in the (lattice) Gibbs-non-Gibbs transition scenario. This "trajectory-large- deviation approach" has then been studied in more generality, including the lattice case, in [4].

In this paper, we apply the trajectory-large-deviation approach in several examples, both for diffusion processes and for birth and death processes. This leads to new and explicitly computable Gibbs-non-Gibbs transitions of mean-field type. For processes of diffusion type, we first treat an explicit example for the rate function of the initial measure, and as dynamics Brownian motion with small variance or the Ornstein-Uhlenbeck process. In all cases, we obtain the explicit form of the conditioned trajectories, and explicit formulas for the bad configuration and the time at which it becomes bad. In the case of general Markovian diffusion processes in a symmetric potential landscape, we show under reasonable conditions short-time Gibbsianness as well as appearance of bad configurations at large times. Next, we treat the case of continuous-time random walk with small increments, as arises e.g. naturally in the context of (properly rescaled) population dynamics. In that case, the Euler-Lagrange trajectories can be explicitly computed for some particular choices of the "birth and death" rates. Constant birth and death rates are the analogue of the Brownian motion case, whereas linear birth and death rates are the analogue of the Ornstein-Uhlenbeck process, but in that case the cost of optimal trajectories becomes a much more complicated expression.

Our paper is organized as follows. In section 3.2 we introduce some elements or the Feng-Kurtz formalism, and define the notion of bad configurations in the present setting. In section 3.3 we treat diffusion processes with small variance, with an explicit form for the initial rate function. In section 3.3.3 we treat the case of Brownian motion dynamics with different cases for the rate function of the initial measure. Finally, in section 3.5, we treat one-dimensional random walks with small increments, such as rescaled birth and death processes.

3.2 The Feng-Kurtz scheme, Euler-Lagrange trajectories, bad configurations

We study Markov processes $\{X_t^n : 0 \leq t \leq T\}$ taking values in $\mathbb{R}^d$, parametrized by a natural number n. This parameter tunes the "amount of noise" in the process, i.e., as $n \to \infty$, the process becomes deterministic, and the measure on trajectories satisfies the

large deviation principle with rate n and with a rate function of the form

$$\mathcal{I}(\gamma) = \int_0^T L(\gamma_s, \dot{\gamma}_s) ds \tag{3.2.1}$$

This means more precisely that

$$\mathbb{P}\left(\{X_t^n : 0 \leq t \leq T\} \approx \gamma\right) \approx \exp\left(-n\mathcal{I}(\gamma)\right) \tag{3.2.2}$$

to be interpreted in the usual sense of the large deviation principle with a suitable topology on the set of trajectories. The form (3.2.1) naturally follows from the Markov property.

Notice that the form of the rate function does not depend on the choice of this topology. So one usually starts with the weakest topology, i.e., the product topology, and then, if possible, strengthens the topology by showing exponential tightness. See [1] for an illustration of this strategy in the context of theorems like Mogulskii's theorem.

Since in this paper we are only interested in finding out optimal trajectories, i.e., minimizers of the rate function over a set of trajectories with prescribed terminal condition and open-start condition, we will not have to worry about the strongest topology in which the large deviation principle (3.2.2) holds, but we are rather after (as explicit as possible) solutions of Euler-Lagrange problems associated to the rate function.

In [8] a scheme is given to compute the "Lagrangian" L, see also [4] for an illustration of this scheme in the large-deviation view on Gibbs-non-Gibbs transitions. First one computes the "Hamiltonian"

$$\mathcal{H}(p, x) = \lim_{n\to\infty} \frac{1}{n} e^{-n\langle p,x\rangle} \mathcal{L}_n e^{n\langle p,x\rangle} \tag{3.2.3}$$

where $\mathcal{L}_n$ is the generator of the process $\{X_t^n : 0 \leq t \leq T\}$ (working on the x-variable), where $p \in \mathbb{R}^d$ is the "momentum" and where $< ., . >$ denotes inner product. Under regularity conditions on $\mathcal{H}(p, x)$ (e.g. strict convexity), the associated Lagrangian is then given by the Legendre transform

$$L(x, v) = \sup_{p\in\mathbb{R}^d} \left(< v, p > -\mathcal{H}(x, p)\right), \tag{3.2.4}$$

As an example, consider

$$X_t^n = n^{-1/2} B_t$$

with generator

$$\mathcal{L}_n = \frac{1}{2n}\Delta$$

then we have

$$\mathcal{H}(x, p) = \frac{p^2}{2}$$

and associated Lagrangian

$$L(x, v) = \frac{v^2}{2}$$

which produces the rate function of the well-known Schilder's theorem

$$\mathbb{P}\left(\{X_t^n : 0 \le t \le T\} \approx \gamma\right) \approx \exp\left(-\frac{n}{2}\int_0^T \dot{\gamma}_s^2 ds\right)$$

To proceed, we also want the initial point of our process to have some fluctuations. More precisely, we need for the starting point of our process an initial measure μ_n (depending on n) on $\mathbb{R}^d$, satisfying the large deviation principle with rate n and rate function $i(x)$, i.e., in the sense of large deviations, we assume

$$\mathbb{P}\left(X_0^n \in A\right) = \mu_n(A) \approx \exp(-n \inf_{x\in A} i(x)) \tag{3.2.5}$$

We call the triple $(\{X_t^n : 0 \le t \le T\}, L, i)$ a stochastic system with small noise.

We continue now with the definition of a bad configuration in this framework. This is motivated by the definition of a bad configuration in the context of mean-field models [10], and can be viewed as the large-deviation rephrasing of "a phase transition at time zero conditioned on a special configuration at time T".

Definition 1. *Let $(\{X_t^n : 0 \le t \le T\}, L, i)$ be a stochastic system with small noise. We say that a point $b \in \mathbb{R}^d$ is bad at time T if the following two conditions hold.*

1. *Conditional on $X_T^n = b$, X_0^n does not converge (as $n \to \infty$) to a point-mass in distribution.*
2. *There exist two sequences $b_k^+ \to b$, $b_k^- \to b$ and $\delta > 0$ such that the variational distance between the distribution $\mu(0, T; b_k^+)$ of $X_0^n | X_T^n = b_k^+$ and the distribution $\mu(0, T; b_k^-)$ of $X_0^n | X_T^n = b_k^-$ is at least δ for k large enough.*

The simplest example which follows also the most common scenario is where the distribution of $X_0^n | X_T^n = b$ converges to $\frac{1}{2}(\delta_{-a} + \delta_a)$ and for $c > b$ $X_0^n | X_T^n = c$ converges to $\delta_{\alpha(c)}$ where $\alpha(c) \to a$ as $c \downarrow b$, whereas for $c < b$ $X_0^n | X_T^n = c$ converges to $\delta_{\alpha'(c)}$ where $\alpha'(c) \to -a$ as $c \uparrow b$. This means that conditioned to be at time T at location b, the process has two "favorite" initial spots, which can be "selected" by approaching b from the right or from the left.

This is the analogue of a phase transition, where the phases can be selected by appropriately approximating the bad configuration, see [3].

3.3 Diffusion processes with small variance conditioned on the future

In this section we present examples where X_t^n is a diffusion process. We show also how from the large deviation approach we gain a new understanding of "short-time Gibbsianness" for a general class of drifts of the diffusion, or initial rate functions.

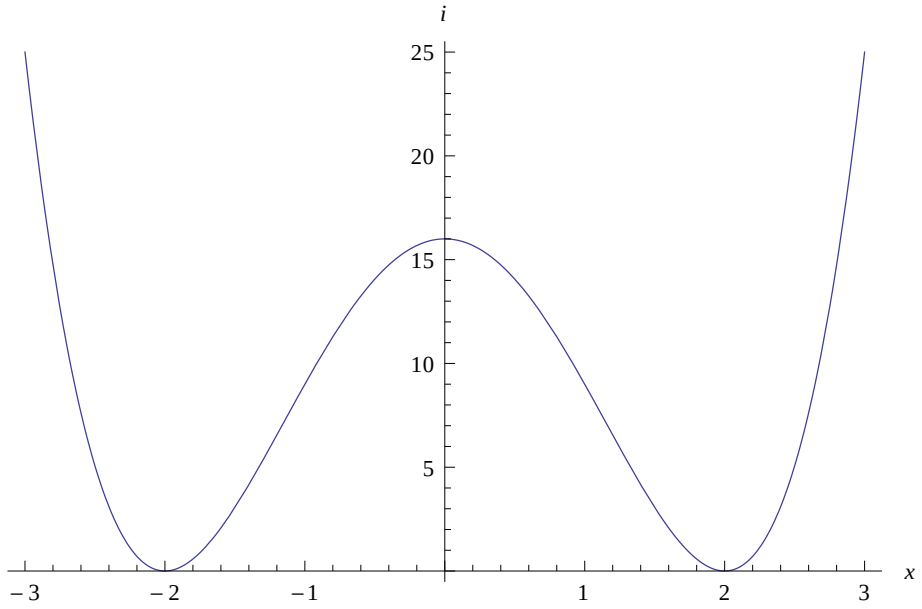

Figure 3.1: $i(x) = (x^2 - a^2)^2$ with $a = 2$

3.3.1 Brownian motion

To start with, we consider Brownian motion with small variance $\frac{1}{n}$ starting from an initial distribution satisfying the large deviation principle (with rate n) with a non-convex rate function having two mimina at locations $-a, a$, with $a > 0$. More precisely, we consider the process

$$X_t^n = \frac{1}{\sqrt{n}} B_t \tag{3.3.1}$$

starting from an initial distribution μ_n such that, informally written,

$$\mathbb{P}\left(X_0^n \in dx\right) = \mu_n(dx) \approx e^{-ni(x)} dx \tag{3.3.2}$$

For i we make the explicit choice:

$$i(x) = (x^2 - a^2)^2 \tag{3.3.3}$$

i.e., a non-convex function, non-negative, with zeros at $-a, a$ and maximum at $x = 0$ ($i(x)$ with $a = 2$ is plotted in Figure 3.1).

This specific choice is for the sake of *explicit analytic computability* but many results are true for a general class of rate functions that have a similar graph with two zeros located at $-a, a$ and a maximum at zero.

More formally, we require that the sequence of initial probability measures $\{\mu_n, n \in \mathbb{N}\}$ satisfies the large deviation principle with rate function i given by (3.3.3). Such rate

functions arise naturally in the context of mean-field models with continuous spins and spin-Hamiltonian depending on the magnetization.

We are then interested in the most probable trajectory γ with initial point distributed according to μ_n and final point $\gamma_T = 0$. More precisely, by application of Schilder's theorem, the trajectory $\{X_t^n : 0 \leq t \leq T\}$ satisfies the LDP with rate function

$$\mathcal{I}(\gamma) = \frac{1}{2}\int_0^T \dot{\gamma}_s^2 ds + i(\gamma_0) \tag{3.3.4}$$

The optimal trajectory we are looking for is hence

$$\arg\min\{\mathcal{I}(\gamma) : \gamma(T) = 0\}$$

The Euler-Lagrange trajectories (extrema of the cost $\frac{1}{2}\int_0^T \dot{\gamma}_s^2 ds$ corresponding to $\mathcal{I}(\gamma)$) are linear in t:

$$\gamma_t = A + Bt$$

By the terminal condition $\gamma_T = 0$, we have $B = -A/T$.

The cost $\mathcal{I}(\gamma)$ of this trajectory can then be rewritten as a function of the starting point $\gamma_0 = A$:

$$\mathcal{E}_{0,T}(A) := \mathcal{I}(\gamma) = A^4 - 2a^2A^2 + a^4 + \frac{1}{2}(-A/T)^2 T = A^4 + \alpha(a,T)A^2 + a^4 \tag{3.3.5}$$

with

$$\alpha(a,T) = \left(\frac{1}{2T} - 2a^2\right) \tag{3.3.6}$$

The behavior of this cost depends on the sign of α. If $\alpha \geq 0$, then there is a unique minimum at $A = 0$, this case corresponds to

$$T \leq \frac{1}{4a^2} := T_{crit}$$

If $\alpha < 0$ then there are two mimima $A = A_\pm$ given by

$$A_\pm = \pm\sqrt{-\alpha(a,T)/2} = \pm\sqrt{a^2 - (4T)^{-1}} \tag{3.3.7}$$

We thus conclude that, as $n \to \infty$, the starting point is most probably 0 for small T and most (and equally) probably $A_\pm$ for large T, which converges to $\pm a$ when $T \to \infty$. Hence we have non-uniqueness of histories.

Let us denote $\mu(n,T,0)$ the distribution of X_0^n conditioned on $X_T^n = 0$. Then we have

1. Small times, unique history. If $T \leq T_{crit}$ then

$$\lim_{n\to\infty} \mu(n,T,0) = \delta_0.$$

2. Large times, non-unique history. If $T > T_{crit}$ then
$$\lim_{n\to\infty} \mu(n, T, 0) = \frac{1}{2}(\delta_{A^+} + \delta_{A^-}).$$

3. Limit of large times
$$\lim_{T\to\infty} \lim_{n\to\infty} \mu(n, T, 0) \to \frac{1}{2}(\delta_a + \delta_{-a}).$$

Let us now condition on $X_T^n = b \neq 0$. Then the most probable trajectory is still a straight line $\gamma_t^b = A + Bt$ but now with terminal condition $A + BT = b$, i.e., $B = (b - A)/T$. It has cost expressed in terms of the starting point $\gamma_0 = A$
$$\mathcal{E}_{b,T}(A) = A^4 + \alpha(a, T)A^2 + a^4 - \frac{b}{T}A + \frac{b^2}{2T} \tag{3.3.8}$$
This is the cost function $\mathcal{E}_{0,T}(A)$ of (3.3.5) plus a linear term $-\frac{b}{T}A + \frac{b^2}{2T}$. Minimization of $\mathcal{E}_{b,T}(A)$ leads to the equation
$$4A^3 + 2\alpha A = \frac{b}{T} \tag{3.3.9}$$

We then have two cases:

1. $\alpha \geq 0$, i.e., $T \leq T_{crit}$. Equation (3.3.9) has a unique real solution, corresponding to a unique minimum A_b of $E_b(A)$. This minimum converges to zero as $b \to 0$. Hence, 0 is good for $T \leq T_{crit}$.

2. $\alpha < 0$. Equation (3.3.9) has three real solutions. For $b > 0$ we have one positive and two negative solutions. The positive solution denoted $A(+, b, T) > \sqrt{-\alpha/2}$ gives the minimum. The negative solutions correspond to a maximum and a local minimum. For $b < 0$ the situation is exactly the opposite: the unique negative solution $A(-, b, T) < -\sqrt{-\alpha/2}$ correspond to the global minimum whereas the two positive solutions give a maximum and a local minimum. Hence 0 is bad for all $T > T_{crit}$

In particular, for the $T \to \infty$ the positive, resp. negative minimum of the rate function of the distribution at time zero is selected by taking the right or left limit of the conditioning.
$$\lim_{c\to 0, b>0} \lim_{T\to\infty} \mathbb{P}(X_0^n = \cdot | X_T^n = c) = \delta_a$$
and, similarly
$$\lim_{c\to 0, b<0} \lim_{T\to\infty} \mathbb{P}(X_0^n = \cdot | X_T^n = c) = \delta_{-a}$$

Summarizing our findings, let us denote $\mathcal{B}_T$ the set of bad configurations then we have

Theorem 1. *1. Short times: no bad configurations.*

For $T \leq \frac{1}{4a^2}$, $\mathcal{B}_T = \varnothing$.

2. Large times: unique bad configuration. For $T > \frac{1}{4a^2}$, $\mathcal{B}_T = \{0\}$

3.3.2 Brownian motion with constant drift

The case of Brownian motion with constant drift $V > 0$ is treated similarly. The Euler-Lagrange trajectories are once more linear in t, but the cost is now

$$i(\gamma_0) + \frac{1}{2}\int_0^T (\dot{\gamma}_s - V)^2 ds$$

which for $\gamma_t = A + Bt$ ending in $\gamma_T = b$ can be computed explicitly and gives

$$E_{b,V}(A) = \frac{1}{2}\left(\frac{b-A}{T} - V\right)^2 + i(A)$$

of which a similar analysis can be given. In particular, choosing $b = VT$ we see that the cost is identical to the zero drift case conditioning to be at zero at time T, and hence this is a bad point for $T > T_{crit}$, where T_{crit} is the same critical time as for the zero drift case. The analysis around this bad point is identical. Notice that the "limiting deterministic dynamics" is $\dot{x} = V$ and the bad point $x_{spec} = VT$ is precisely where this dynamics ends up at time T when started from zero.

3.3.3 Other rate functions for the initial measure and corresponding behavior of Brownian motion

We now consider other possible scenarios for different rate functions associated to the initial measure, and for the Brownian motion with small variance as dynamics. The starting measure $\mu_n(dx)$ satisfies the large deviation principle with rate function $i(x)$. As a consequence, the minimizing trajectory to arrive at position b at time T is $\gamma_t = Bt + A$ with $B = (b - A)/T$ and has cost

$$\mathcal{E}_{b,T}(A) = \frac{(b-A)^2}{2T} + i(A) \tag{3.3.11}$$

The following scenarios can then occur

1. $i(A)$ **is strictly convex: no bad configurations.** Indeed, in that case $\mathcal{E}(A)$ is also strictly convex (as a sum of two strict convex function) and hence has a unique minimum. In this scenario, there are no bad configurations, and the optimal conditioned trajectory is always unique. This corresponds to "high-temperature initial measure" and "infinite-temperature dynamics", which always conserves Gibbsianness.

2. **Initial field: loss without recovery, with a "compensating" bad configuration.** As an example we can take $i(A) = (A^2 - a^2)^2 + A + r$. For $a > 1$, this rate function has one local minimum in the vicinity of $x = a$, a maximum in the vicinity

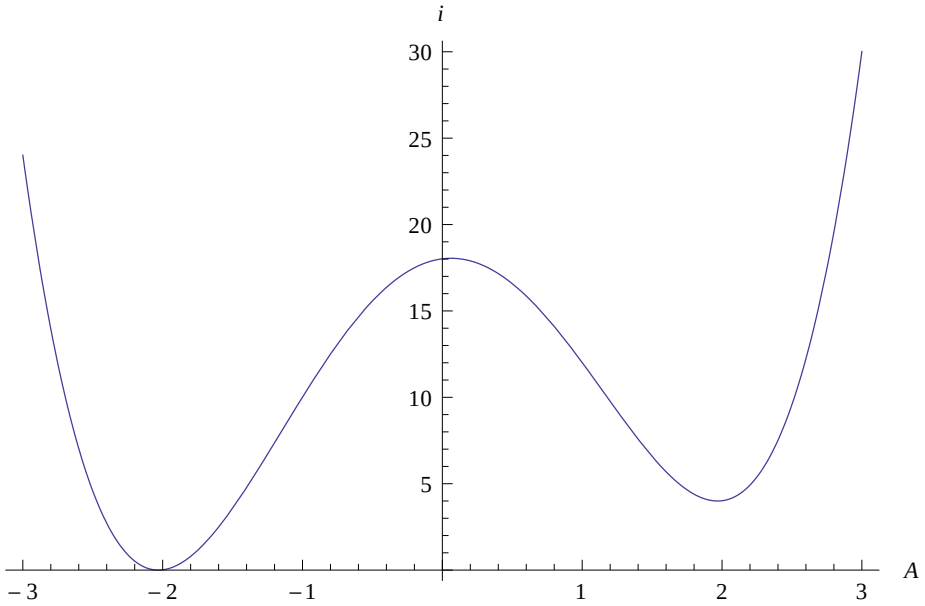

Figure 3.2: $i(A) = (A^2 - a^2)^2 + A + r$ with $a = 2$ and $r = 2.01539$

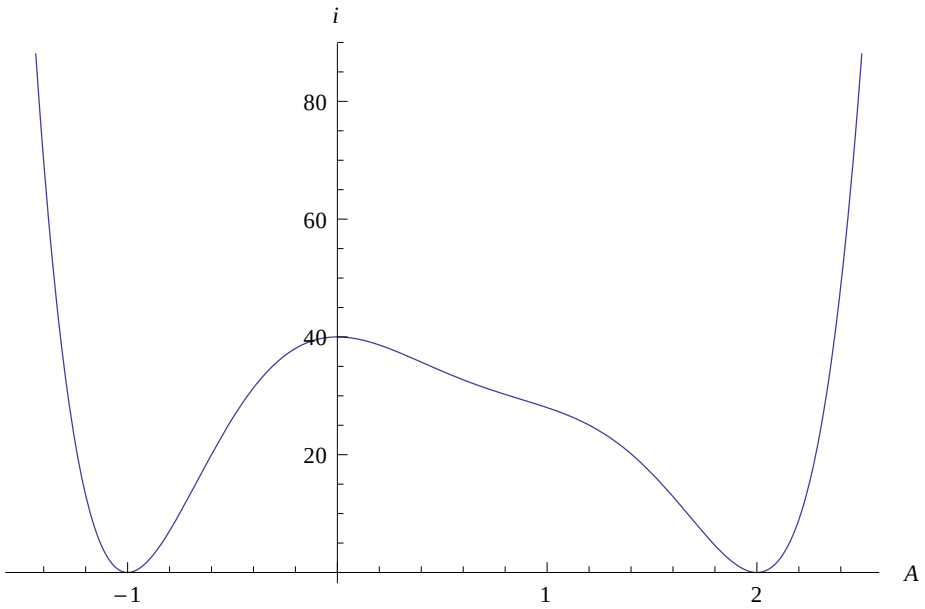

Figure 3.3: $i(A) = 7A^6 - 24A^5 + 9A^4 + 38A^3 - 42A^2 + 40$

of $x = 0$ and its (absolute) minimum in the vicinity of $x = -a$. This corresponds to an initial field (favorizing the minimizer $x = -a$). $i(A)$ with $a = 2$ with $r = 2.01539$ is plotted in Figure 3.2. The minimization of $\mathcal{E}_{b,T}(A)$ leads to the equation

$$4A^3 + 2\alpha(a,T)A = \frac{b}{T} - 1 \tag{3.3.12}$$

By an analysis of (3.3.12) similar for (3.3.9), we obtain that there is no bad point when $T \leq T_{crit} = \frac{1}{4a^2}$, but $b = T$ is bad for all $T > T_{crit}$. The bad point "compensates" the initial field, and therefore has to become larger (and positive) when time T increases.

3. **Non-symmetric rate function.** To see that the symmetry of the initial rate function is not a necessary requirement to produce bad configurations, we have the following example. Let $i(A) = 7A^6 - 24A^5 + 9A^4 + 38A^3 - 42A^2 + 40$ (see Figure 3.3). This rate function has two global minima at $A = -1$ and $A = 2$ and one maximum at $A = 0$. The cost function corresponding to trajectories arriving at b at time T is

$$\mathcal{E}_{b,T}(A) = 7A^6 - 24A^5 + 9A^4 + 38A^3 + \left(\frac{1}{2T} - 42\right)A^2 - \frac{b}{T}A + \frac{b^2}{2T} + 40$$

For fixed b, and T large enough, this function has two local minima, located at $A^1(b,T) < A^2(b,T)$. Let us denote, for fixed T,

$$D_T(b) = \mathcal{E}_{b,T}(A^1(b,T)) - \mathcal{E}_{b,T}(A^2(b,T))$$

If as a function of b, D_T changes sign, by continuity, there must be a value of b^* where $D_T(b^*) = 0$, i.e., where the minima of $\mathcal{E}_{b^*,T}$ are at equal height. This b^* is then a bad point at time T. For $T = 1$ we have $D_T(0.499) \approx -0.00182497 < 0$ and $D_T(0.4999) \approx 0.000868034 > 0$, so at $T = 1$, there is a bad point at $b^* \in (0.499, 0.4999)$. We observe that b^* is T dependent and tends to 0.5 as T increases. From numerical computation, we have $b^* \in (0.4999, 0.49999)$ for $T = 4$, $b^* \in (0.49999, 0.499999)$ for $T = 39$ and $b^* \in (0.499999, 0.4999999)$ for $T = 1000$.

4. **General symmetric rate function.** For *any rate function $i(A)$ which is symmetric with respect to $x = 0$* and which has minima for $A \neq 0$, $b = 0$ is bad when T is large enough. Indeed, the cost to arrive at 0 is from (3.3.11): $i(A) + \frac{A^2}{2T}$ which has a non zero minimum as soon as T is large enough.

5. **General short-time Gibbsianness.** For *every rate function i which is twice differentiable and its second derivative is continuous and bounded from below*, we show that for T small enough there is a unique minimum A_b of $\mathcal{E}_{b,T}(A)$. This is the analogue of "short-time" Gibbsianness obtained in the lattice case via cluster expansions [13] or conditional Dobrushin uniqueness [14] and can be proved as follows.

We look at the equation (see (3.3.11))

$$i'(A) = -\frac{A}{T} + \frac{b}{T} =: f(A). \tag{3.3.13}$$

Put $d = \inf_A i''(A)$. Then we conclude, for

$$T < -\frac{1}{d}, \tag{3.3.14}$$

that (3.3.13) has only one real solution A_b. Indeed, look at any two adjacent intersection points A_1 and A_2 of $i'(A)$ and $f(A)$ if there were more than one real solution for (3.3.13). By the intermediate value theorem, we get

$$\min(i''(A_1), i''(A_2)) < -\frac{1}{T} < d = \inf_A i''(A). \tag{3.3.15}$$

This is a contradiction. And further because $i''(A_b) > -\frac{1}{T}$, we have

$$\mathcal{E}''_{b,T}(A_b) = i''(A_b) + \frac{1}{T} > 0. \tag{3.3.16}$$

Therefore A_b is a minimum.

Remark 2. *In order to understand better the connection between our large deviation based notion of badness, and badness in the sense of conditional probabilities in the mean-field setting, we first remark that the initial measure $\mu_n(x) \approx e^{-ni_0(x)}dx$ can be produced as follows.*

Start from an independent standard normal a-priori measure on $\mathbb{R}^n$

$$\alpha_n(dx_1, \ldots, dx_n) = \prod_{i=1}^{n} \frac{e^{-\frac{1}{2}x_i^2}}{\sqrt{2\pi}} dx_i$$

Under this measure α_n, the "average magnetization" $\overline{x}_n = (1/n)\sum_{i=1}^n x_i$ satisfies the large deviation principle with rate function $\tilde{\imath}(x) = x^2/2$. If we tilt the a-priori measure α_n with the function $F = F(\overline{x}_n)$, i.e., if we consider the measure

$$\mu_n^F = e^{nF(\overline{x}_n)}\alpha_n(dx_1, \ldots, dx_n)$$

then under μ_n^F, $\overline{x}_n$ satisfies the large deviation principle with rate function $i_F(x) = (\tilde{\imath}(x) - F(x)) - C$ where $C = \inf_x(\tilde{\imath}(x) - F(x))$. Making then the choice

$$F(x) = \frac{x^2}{2} - (x^2 - a^2)^2$$

leads to a measure μ_n^F such that $\overline{x}_n$ satisfies the large deviation principle with rate function (3.3.3).

Next, if we start $(x_, \ldots, x_n)$ from this measure μ_n^F and apply independent Brownian motions $(W_t^1, \ldots, W_t^n)$, then the "magnetization" at time $t > 0$ exactly evolves as the process X_t^n in (3.3.1).

Therefore, if we have at least two optimal trajectories conditioned to arrive at a certain magnetization m^* at time $T > 0$, and these trajectories can be selected by approximating the magnetization appropriately, then we have an essential discontinuity at $m = m^*$ of the conditional distribution $m \mapsto \mu_n^F(t)(dx_1|m)$ as a function of the magnetization $m = (1/n)\sum_{i=2}^n x_i$. Such a discontinuity is referred to as non-Gibbsianness in the mean-field context, see [9], [11] for more details.

3.4 The Ornstein-Uhlenbeck process

As a second example, we consider the process X_t^n to be the solution of

$$dX_t = -\kappa X_t dt + \frac{1}{\sqrt{n}} dB_t$$

and the initial point distributed as in the previous section, in (3.3.2), (3.3.3).

The cost function for the large deviation principle of the trajectories now becomes

$$\mathcal{I}(\gamma) = i(\gamma_0) + \frac{1}{2}\int_0^T (\dot{\gamma}_s + \kappa\gamma_s)^2 ds \tag{3.4.1}$$

The Euler-Lagrange trajectories extremizing $\frac{1}{2}\int_0^T (\dot{\gamma}_s + \kappa\gamma_s)^2 ds$ are given by

$$\gamma_t = Ae^{\kappa t} + Be^{-\kappa t}$$

by the terminal condition $\gamma_T = 0$ we have

$$\gamma_t = -Be^{-2\kappa T}e^{\kappa t} + Be^{-\kappa t}$$

the cost function for such a trajectory can then explicitly be evaluated and gives

$$\mathcal{E}_{0,T}(B) = c_1 B^4 + c_2 B^2 + c_3 \tag{3.4.2}$$

where

$$\begin{aligned} c_1 &= (1 - e^{-2\kappa t})^4 \\ c_2 &= \left(-2a^2(1 - e^{-2\kappa t})^2 + \kappa e^{-2\kappa t}(1 - e^{-2\kappa t})\right) \\ c_3 &= a^4 \end{aligned} \tag{3.4.3}$$

A similar analysis as in the previous section can now be started. We have a unique minimum at $B = 0$ of the cost function $\mathcal{E}$ for

$$T \leq T_{crit} := -\frac{1}{2\kappa}\log\left(\frac{2a^2}{2a^2 + \kappa}\right) \tag{3.4.4}$$

and for $T > T_{crit}$, 0 becomes the unique bad point for this process.

The cost of an optimal trajectory ending up at b at time T can also be expressed as a function of the starting point γ_0, which gives the explicit expression

$$\mathcal{E}_{b,T}(\gamma_0) = i(\gamma_0) + \frac{\kappa}{e^{2\kappa T} - 1}(\gamma_0 - be^{\kappa T})^2 \tag{3.4.5}$$

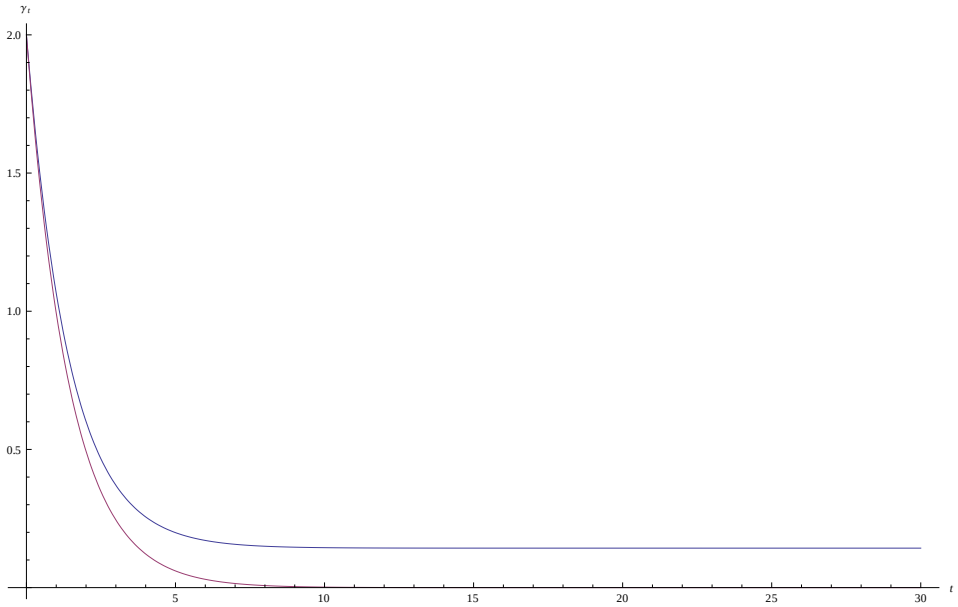

Figure 3.4: A limiting process (the purple line) with $a = 2, \kappa = 0.7, T = 30$, hence $\gamma_0^+ \approx 2.0$, and a corresponding conditioned process (the blue line) with $E = 0.1$, $b \approx 0.142857$

3.4.1 The Ornstein-Uhlenbeck process with constant external field

The equation for the process X_T^n then reads

$$dX_t^n = (-\kappa X_t + E)dt + \frac{1}{\sqrt{n}} dB_t \tag{3.4.6}$$

where $E > 0$ is a constant representing a (constant) external field. As rate function of the initial measure we choose as before (3.3.3). The cost of the trajectory is now given by $\int_0^T L(\gamma_s, \dot{\gamma}_s)ds$ with $L(\gamma_s, \dot{\gamma}_s) = (\dot{\gamma}_s + \kappa\gamma_s - E)^2$. The Euler-Lagrange trajectories are of the form

$$\gamma_t = Ae^{\kappa t} + Be^{-\kappa t} + \frac{E}{\kappa}$$

The trajectory cost of an Euler-Lagrange trajectory is given by $2A^2(e^{2\kappa T} - 1)$. From this, we derive that the total cost of a trajectory to end up at time T in $\gamma_T = b$ is given, as a function of γ_0, by

$$\mathcal{E}_{b,T}^E(\gamma_0) = i(\gamma_0) + \frac{\kappa\left(\gamma_0 - \left(b - \frac{E}{\kappa}\right)e^{\kappa T} - \frac{E}{\kappa}\right)^2}{e^{2\kappa T} - 1}$$

The same analysis can then be performed. The "critical" time at which a unique bad point starts to appear is the same as in the zero-field case, i.e., given by (3.4.4). This bad point is given by

$$b = \frac{E}{\kappa}(1 - e^{-\kappa T}) \tag{3.4.7}$$

which corresponds to the point at which the deterministic evolution $\dot{x}_t = -\kappa x_t + E$ arrives when starting from $x_0 = 0$. Notice that total cost to arrive at this bad point b is given by

$$i(\gamma_0) + \frac{\kappa\gamma_0^2}{e^{2\kappa T} - 1}$$

which is symmetric around $\gamma_0 = 0$. Moreover, for T large the path cost contribution which is equal to $\frac{\kappa\gamma_0^2}{e^{2\kappa T}-1}$ vanishes exponentially fast, and hence for large T two minima exist.

The corresponding optimal trajectories to arrive at the bad point b are starting from

$$\gamma_0^{\pm} = \pm\sqrt{a^2 - \frac{\kappa}{2(e^{2\kappa T} - 1)}}$$

and explicitly given by

$$\gamma_t = \left(b - \frac{E}{\kappa}\right)\frac{\sinh(\kappa t)}{\sinh(\kappa T)} + \left(\gamma_0 - \frac{E}{\kappa}\right)\frac{\sinh(\kappa(T-t))}{\sinh(\kappa T)} + \frac{E}{\kappa}$$

The trajectory with plus resp. minus sign can be selected by conditioning to arrive at $b^+ > b$, resp. $b^- < b$, and letting $b^+ \to b$, resp. $b^- \to b$. Here we plot a limiting process with $a = 2, \kappa = 0.7, T = 30$, hence $\gamma_0^+ \approx 2.0$, and a corresponding conditioned process with $E = 0.1$, hence $b \approx 0.142857$, see Figure 3.4.

3.4.2 General drift.

Let us now consider the process X_t^n with a general drift $f(x)$ and variance $\frac{1}{n}$, i.e., the solution of

$$dX_t = -f(X_t)dt + \frac{1}{\sqrt{n}}dB_t$$

We assume $f : \mathbb{R} \to \mathbb{R}$ to be Lipschitz, and odd: $f(-x) = -f(x)$. For the rate function of the initial point X_0^n we choose as before (3.3.2), (3.3.3). The rate function of the trajectory is now given by

$$\mathcal{I}(\gamma) = \frac{1}{2}\int_0^T (\dot{\gamma}_s + f(\gamma_s))^2 ds \tag{3.4.8}$$

and the minimization problem for the optimal trajectory ending at zero $\gamma_T = 0$ becomes now to find

$$\arg\min\{\mathcal{I}(\gamma) + i(\gamma_0) : \gamma_T = 0\} \tag{3.4.9}$$

The Euler-Lagrange equations for miminal cost trajectories are given by

$$\frac{d^2\gamma_s}{ds^2} = f(\gamma_s)f'(\gamma_s)$$

These equations correspond to classical motion in a potential U satisfying $U' = -ff'$, which gives as a possible choice $U = -\frac{1}{2}f^2$. Notice that this formal potential U has no physical

meaning, but we need it if we want to translate the framework of the Euler-Lagrange equations to Hamilton equations. Indeed, the corresponding Hamiltonian is

$$H(p,q) = \frac{p^2}{2} - U(q) \tag{3.4.10}$$

In particular, under the Euler-Lagrange equations,

$$\frac{\dot{\gamma}_t^2}{2} - \frac{1}{2}(f(\gamma_t))^2 = E \tag{3.4.11}$$

is a constant of motion. Further, we have the open-start and terminal condition

$$\begin{aligned} i'(\gamma_0) &= \dot{\gamma_0} + f(\gamma_0) \\ \gamma_T &= 0 \end{aligned} \tag{3.4.12}$$

We can think of these equations as having γ_0 and E as parameters. The terminal condition gives then a relation between E and γ_0. Notice that the trajectory of zero-energy, $E = 0$, $\gamma \equiv 0$ is always a solution since $f(0) = 0$. We want to show that under some reasonable assumptions, for T small, it is the only solution. For this we make the following assumptions. Call $\mathcal{S}_T(E)$ the collection of all trajectories $\gamma : [0,T] \to \mathbb{R}$ ending at 0, i.e., with $\gamma_T = 0$ and with "energy" E, i.e., such that

$$\frac{\dot{\gamma}_t^2}{2} - \frac{1}{2}(f(\gamma_t))^2 = E$$

for all $0 \leq t \leq T$. We impose now the following conditions.

1. There exist a function $\varphi : \mathbb{R} \to [0,\infty)$ and $T_0 > 0$ and a constant $C > 0$ such that $\varphi(0) = 0$, $\varphi(E) > 0$ for $E \neq 0$ such that for all $T \leq T_0$ and for all $\gamma \in \mathcal{S}_T(E)$, $\gamma_0\dot{\gamma}_0 < 0$,

$$|\dot{\gamma}_0| \geq \varphi(E) \tag{3.4.13}$$

and

$$|\gamma_0| \leq C\varphi(E)T \tag{3.4.14}$$

2. The drift function f is locally monotone around 0, i.e., there exist x_0 such that f restricted to $[0,x_0]$, $[-x_0,0]$ is monotone.

The first condition states that if T is small, and one wants to end at $\gamma_T = 0$ from $\gamma_0 > 0$, then the derivative at zero should be negative, or vice versa. The second part of the condition states that there exist lower bounds for the derivative and upper bounds for γ_0.

Coming back to the previous examples: for the Brownian motion case, for all $\gamma \in \mathcal{S}_T(E)$ we have $\gamma_t = \pm\sqrt{2E}(t-T)$ hence and for $\gamma \in \mathcal{S}_T(E)$ we have $\gamma_0 = \mp\sqrt{2E}T$,

$\dot\gamma_0 = \pm\sqrt{2E}$, and we can choose $\varphi(E) = \sqrt{2E}$. For the Ornstein-Uhlenbeck case we have $\gamma_t = B(e^{-\kappa t} - e^{-\kappa(2T-t)})$, $E = -2AB\alpha$ and if $\gamma_T = 0$ we find $\gamma_0 = \sqrt{2E/\kappa}\sinh(\kappa T)$, $\dot\gamma_0 = -\sqrt{2E/\kappa}\cosh(\kappa T)$ which clearly satisfies the conditions, with the $\varphi = \sqrt{2E/\kappa}$.

The open-start condition requires

$$\dot\gamma_0 + f(\gamma_0) = 4\gamma_0(\gamma_0^2 - a^2)$$

Hence, for $\gamma \in \mathcal{S}_T(E)$ such that $\gamma_0 > 0$:

$$\begin{aligned} -\varphi(E) &\geq \dot\gamma_0 \\ &\geq 4\gamma_0(\gamma_0^2 - a^2) - f(C\varphi(E)T) \\ &\geq 4C\varphi(E)T(C^2\varphi(E)^2T^2 - a^2) - f(C\varphi(E)T) \end{aligned} \tag{3.4.15}$$

which is clearly a contradiction for T sufficiently small. Hence for T sufficiently small, there do not exist $E \neq 0$ with $\gamma \in S_T(E)$. As a consequence, under these assumptions, for small T the zero trajectory is the only solution of the minimization problem (3.4.9).

For large times, if we assume that the drift is such that from any starting point one can travel to the origin at arbitrary small cost if one has sufficient time, i.e., for all $x_0 > 0$,

$$\lim_{T\to\infty} \inf\left\{\int_0^T (\dot\gamma_s + f(\gamma)_s)^2 ds : \gamma_0 = x_0, \gamma_T = 0\right\} = 0$$

then this implies that for T large enough that there exists $x_0 \neq 0$ and a trajectory γ starting from x_0 such that $i(x_0) < i(0)/2$ and

$$\left\{\int_0^T (\dot\gamma_s + f(\gamma)_s)^2 ds : \gamma_0 = x_0, \gamma_T = 0\right\} < i(0)/2$$

this trajectory γ clearly has lower cost than the zero trajectory, and by symmetry, $-\gamma$ is a trajectory with identical cost. Therefore, 0 becomes a bad point.

3.5 Approximately deterministic walks in $d = 1$

An "approximately deterministic random walk" is a continuous-time random walk with small increments performed at high rate, i.e., a random walk X_t^N on $\mathbb{R}$ that, starting at $X_0 = x$, makes increments of size $\pm 1/N$ with rates $Nb(x)$, resp. $Nd(x)$. In other words, X_t^N is a Markov process on $\mathbb{R}$ with generator

$$\mathcal{L}_N f(x) = Nb(x)\left(f\left(x + \frac{1}{N}\right) - f(x)\right) + Nd(x)\left(f\left(x - \frac{1}{N}\right) - f(x)\right) \tag{3.5.1}$$

Such walks arise naturally in the context of population dynamics, see e.g. [7]. The notation $b(x)$ and $d(x)$ is also reminiscent of this interpretation and we will call these quantities birth resp. death rates.

We ask then the same large deviation question, i.e., we start the process X_t^N from an initial distribution μ_N satisfying the large deviation principle with rate function (3.3.3) - or some natural modification of it if we have to restrict the state space- and look for the minimizing trajectory(ies) that end at time T at the origin (or at a more general bad point if the dynamics has a drift, see later).

The large deviation function for the trajectories can be computed using the Feng-Kurtz scheme, i.e., denoting $f_p^N(x) = e^{Npx}$ we compute the Hamiltonian

$$\mathcal{H}(x,p) = \lim_{N\to\infty} \frac{1}{N}\left(\frac{1}{f_p^N}(\mathcal{L}_N f_p^N)\right)(x) = (e^p - 1)b(x) + (e^{-p} - 1)d(x) \tag{3.5.2}$$

and the corresponding Lagrangian

$$L(x,v) = \sup_{p\in\mathbb{R}} (pv - \mathcal{H}(x,p)) \tag{3.5.3}$$

For the trajectories of $\{X_t^N : 0 \le t \le T\}$, we have

$$\mathbb{P}(X_\cdot^N \approx \gamma) \approx e^{-N\int_0^T L(\gamma_s,\dot\gamma_s)ds} \tag{3.5.4}$$

where the informal notation has to be interpreted as usual in the sense of the large deviation principle.

The equations for the optimal trajectories, i.e. for the minimizers of the "action"

$$\mathcal{I}(\gamma) = i(\gamma_0) + \int_0^T L(\gamma_s,\dot\gamma_s)ds \tag{3.5.5}$$

can now more conveniently be written in terms of the Hamiltonian (the Lagrangian is a more complicated expression to deal with).

Introducing the canonical coordinates (x,p) we have the Hamilton equations, together with the terminal condition and the open-start condition corresponding to the choice of the distribution of X_0^N.

$$\begin{aligned} \dot x_t &= \frac{\partial H}{\partial p}(x_t,p_t) = b(x)e^p - d(x)e^{-p} \\ \dot p_t &= -\frac{\partial H}{\partial x}(x_t,p_t) = -b'(x)(e^p-1) - d'(x)(e^{-p}-1) \end{aligned} \tag{3.5.6}$$

with conditions

$$\begin{aligned} x_T &= 0 \\ p_0 &= i'(x_0) = 4x_0(x_0^2 - a^2) \end{aligned} \tag{3.5.7}$$

Where i_0 is the quartic rate function from (3.3.3). The total "energy" is a constant of motion along minimizing trajectories, so we put $H(x,p) = E$ and we can rewrite the Hamilton equations (3.5.6)

$$\begin{aligned} E + b(x) + d(x) + \dot{x} &= 2b(x)u \\ E + b(x) + d(x) - \dot{x} &= 2d(x)u^{-1} \end{aligned} \tag{3.5.8}$$

where $u = e^p$. This leads to

$$\dot{x}^2 = E^2 + 2E(b(x) + d(x)) + (b(x) - d(x))^2 \tag{3.5.9}$$

So we can think now of the cost of a trajectory as a function of two parameters: the starting point and the energy (x_0, E). Zero-energy correspond to the "typical trajectory" following the limiting differential equation $\dot{x} = b(x) - d(x)$, which means that the cost of the Lagrangian part of the rate function is zero, and only the cost due to the starting point x_0 has to be paid. Non-zero energy trajectories have a strictly positive cost of the Lagrangian part of the rate function. The additional terminal condition $X_T = b$ will eliminate one of these variables (e.g. E), so that we can think of the cost of the trajectory as a function of a single variable (e.g. x_0).

We now concentrate on three important particular cases.

3.5.1 Constant birth and death rates

If b and d do not depend on x, then the equation for the momentum shows that $p_t = C$, hence we have linear Euler-Lagrange trajectories, and correspondingly the same analysis and phenomena as in the Brownian motion case of the previous section.

3.5.2 Mean-field independent spin flips

A special case, corresponding to independent spin-flip dynamics is $b(x) = (1 - x)$, $d(x) = (1 + x)$. Moreover, the x-variable is now restricted to $[-1, 1]$. As in the case $x \in \mathbb{R}$ we assume that initially, x_0 is distributed according to a measure $\mu_n(dx)$ on $[-1, 1]$ satisfying the large deviation principle with the non-convex rate function (3.3.3) for $x \in [-1, 1]$ and $+\infty$ otherwise. In particular, $a \in (0, 1)$.

The Hamilton equations then read

$$\begin{aligned} \dot{x} &= -x(e^p + e^{-p}) + e^p - e^{-p} \\ \dot{p} &= e^p - e^{-p} \end{aligned} \tag{3.5.10}$$

Taking the derivative w.r.t. time of the first equation and using the second equation leads to elimination of p, and the simple second order equation for x: to

$$\frac{d^2x}{dt^2} = 4x \tag{3.5.11}$$

with solutions

$$x(t) = C_1 e^{2t} + C_2 e^{-2t}$$

where C_1, C_2 are determined by the open-start condition and the terminal condition. This case was treated before in the context of the Curie-Weiss model subjected to independent spin flips in [10], [13].

The equation for the momentum can be integrated and gives

$$\tanh(p_t/2) = \pm C e^{2t}$$

Furthermore, since

$$E = (1-x)(e^p - 1) + (1+x)(e^{-p} - 1)$$

is a constant of motion, we find as possible solutions for x, using that $x_T = 0$:

$$x_t = \pm\sqrt{E/4(1+E/4)}\left(e^{2(t-T)} - e^{2(T-t)}\right)$$

In particular, as in the Brownian motion case, the zero-energy trajectory ($E = 0$) yields $x_t = 0$. The relation between the energy, initial position and initial momentum is

$$p_0 = \log\left(\frac{2 + E + \sqrt{(2+E)^2 - 4(1-x_0^2)}}{2(1-x_0)}\right)$$

Zero-energy thus corresponds to zero initial momentum and zero initial position.

In general, the initial points are symmetrically distributed around the origin and related to the energy via

$$x_0 = \pm\sqrt{E/4(1+E/4)}\left(e^{-2T} - e^{2T}\right)$$

Whether or not a non-zero energy solution can be the minimizer is determined by the open-start condition:

$$p_0 = i'(x_0) = 4x_0(x_0^2 - a^2) \tag{3.5.12}$$

This can be viewed now as an equation for E. For small $T > 0$,

$$x_0 = x_0(E,T) \approx C(E)T, p_0 = p_0(E,T) \approx cE$$

which implies that a non-zero energy solution of (3.5.12) can not exist for small T. For large T, a non-zero energy solution exists, yielding two symmetrically solutions for x_0.

Alternatively, the trajectory cost $C_T(\gamma_0)$ of a trajectory starting at γ_0 ending up at time T at $b = 0$ has the following important properties

1. Symmetry: $C_T(-\gamma_0) = C_T(\gamma_0)$

2. Small time behavior: $\lim_{T\to 0} C_T(\gamma_0) = \infty$ for all $\gamma_0 \neq 0$

3. Large time behavior: $\lim_{T\to\infty} C_T(\gamma_0) = 0$ for all γ_0

From these properties it follows that for small T there are no bad points, and for large T zero is the unique bad point. Notice that contrary to the Curie-Weiss model situation analyzed in [10] there are no non-neutral (non-zero) bad configurations due to the fact that the rate function of the initial measure is here simply a fourth-order polynomial.

3.5.3 Independent spin-flips in a field

This corresponds to the choice $b(x) = \gamma(1-x)$, $d(x) = (1+x)$, $x \in [-1,1]$. Here $\gamma > 1$ corresponds to a bias in the plus direction (positive magnetic field). The limiting deterministic trajectory is given by

$$\frac{dx_t}{dt} = -(1+\gamma)x_t + (\gamma - 1)$$

$$x_t = x_0 e^{-(1+\gamma)t} + \frac{\gamma - 1}{1+\gamma}\left(1 - e^{-(1+\gamma)t}\right) \tag{3.5.13}$$

This is the zero-energy trajectory starting from x_0.

Using (3.5.9) we find that for a given energy E, the solution for x is of the form

$$x_t = x(E, C, t) = C_1 e^{t(1+\gamma)} + C_2 e^{-t(1+\gamma)} + C_3 \tag{3.5.14}$$

with

$$\begin{aligned} C_1 &= \frac{C(2+2\gamma+E)}{(\gamma+1)^2} \\ C_2 &= \frac{E\gamma}{-C(1+\gamma)^2)} \\ C_3 &= \left(\frac{(E+1+\gamma)(\gamma-1)}{(1+\gamma)^2}\right) \end{aligned} \tag{3.5.15}$$

where C is an integration constant.

Remark 3. *1. Remark that for $E = 0$ $C_3 = (\gamma-1)(1+\gamma)^{-1}$ which corresponds to the limiting value of the zero-energy trajectory.*

2. If $\gamma = 1$, and $E \neq 0$ we find $C_3 = 0$ and recover the solution of the form $C_1 e^{2t} + C_2 e^{-2t}$ corresponding to the optimal trajectories of the independent spin-flip dynamics.

The general form of an optimal trajectory arriving at time T at $x_T = b$ and starting from $x_0 = \gamma_0$ is

$$x(t) = (b - C_3)\frac{\sinh(\delta t)}{\sinh(\delta T)} + (\gamma_0 - C_3)\frac{\sinh(\delta(T-t))}{\sinh(\delta T)} + C_3$$

with $\delta = (1 + \gamma)$ and where C_3 is given in (3.5.15). Notice the analogy with the case of the Ornstein-Uhlenbeck process in a constant field (3.4.7). As in that case, the bad point is time-dependent and given by

$$b = \frac{\gamma - 1}{\gamma + 1}\left(1 - e^{-\delta T}\right)$$

which is the point at which the limiting deterministic dynamics arrives at time T when started from $x_0 = 0$. The trajectory cost $C_T(\gamma_0)$ to arrive at this bad point satisfies the same properties as the trajectory cost $C_T(\gamma_0)$ of the previous subsection (zero-field case). Hence, for T large two minimizing γ_0 of the total cost function appear which correspond to two optimal trajectories.

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4

Large deviations for the trajectory of the empirical distribution and empirical measure

4.1 Introduction

In [3] we started investigating how Gibbs-non-Gibbs transitions in lattice spin systems can be related to a bifurcation phenomenon in the nature of the optimal trajectories of the empirical measure. In [9] such a formalism was developed in the mean-field context, i.e., for the trajectory of the magnetization. The idea to study the trajectory of the empirical measure is that one conditions to arrive at time $T > 0$ at a given empirical measure and at time zero one gives a certain cost to each starting measure. This cost is determined by the choice of the initial Gibbs measure, i.e., equals the relative entropy density w.r.t. the initial Gibbs measure μ. Uniqueness for every conditioning of the empirical measure at time $T > 0$ or non-uniqueness for a particular conditioning of the empirical measure at time T, correspond (roughly speaking) to Gibbsianness or non-Gibbsianness of the distribution μ_T at time T. The total cost to arrive at time $T > 0$ at a given empirical measure is the sum of the initial cost and a path cost, determined by the Markovian dynamics. This path cost is usually of the form of a Lagrangian action. This means, informally written, that the probability of a trajectory of the empirical measure, where one averages shifts of the point mass of the lattice-spin configuration over the box $[-N, N]^d$,is expected to behave as

$$\mathbb{P}\left((\mathbb{L}_N(\sigma_t))_{0\le t\le T} \approx (\mu_t)_{0\le t\le T}\right) \approx \exp\left(-(2N+1)^d \int_0^T \Xi(\mu_s, \dot{\mu}_s)\, ds\right)$$

The Lagrangian $\Xi(\mu_s, \dot{\mu}_s)$ is the object we are after in the present paper.

More precisely, we consider two cases in the present paper.

4. LARGE DEVIATIONS FOR THE TRAJECTORY OF THE EMPIRICAL DISTRIBUTION AND EMPIRICAL MEASURE

First, in the context of independent Markov processes on a general state space E, we study the Lagrangian of the associated to the large deviations of the trajectory of the empirical distribution

$$\mathcal{L}_N = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_t^i}$$

which is a random probability measure on E. We compute explicitly the Hamiltonian and provide some information about the associated Hamiltonian trajectories for finite-state space Markov chains. For diffusion processes, the Lagrangian is a natural quadratic form associated to the generator. For Markov chains, the Lagrangian is less explicit (except for two-state Markov chains), but can still be characterized as a relative entropy production. Moreover, the characterization of minimal action or optimal (w.r.t. path cost) trajectories can be done using the Hamiltonian formalism as well. The study of the large deviations of the trajectory of the empirical distribution has to be considered as the intermediate step between the magnetization (studied in [9]) and the empirical measure. In particular, for finite-state space Markov chains, the empirical distribution is still a finite-dimensional object.

Second, in the context of translation invariant interacting Markov processes, we consider the trajectory of the empirical measure, and compute explicitly the Hamiltonian, both for diffusion processes and for jump processes of interacting particle type. In the context of diffusion processes, the Lagrangian is a quadratic form, while in the context of jump processes (of interacting particle systems type), the Lagrangian is less explicit, but also there a relative entropy production (density) characterization can be given.

This study is a step in the research programme proposed in [3]. Given the Hamiltonians and Lagrangians computed in the present paper, one can then characterize bifurcation phenomena, i.e., non-uniqueness of optimal trajectories for particular choices of initial costs. We leave this problem for future work and focus here on the explicit form of the Hamiltonian and Lagrangian.

Our paper is organized as follows. In section 2 we give a general computation of the Feng-Kurtz Hamiltonian for the trajectory of the empirical distribution. In section 3 we study the case of finite continuous-time Markov chains. In section 4 we consider the case of diffusion processes. In section 5 we consider the case of interacting Markov processes, both of jump type (interacting particle systems in the spirit of [12]) and of diffusion type.

4.2 The trajectory of the empirical distribution: general case

We consider $\{X_t : 0 \leq t \leq T\}$ a (Feller) Markov process on a state space E. We assume E to be a locally compact Polish space. Relevant cases for the present paper are, E a finite set (finite Markov chains), or $E = \mathbb{R}^k$ or a compact submanifold of $\mathbb{R}^k$ (diffusions). The computation of this section is however valid for general E.

We denote by Q the generator of the process $\{X_t : 0 \leq t \leq T\}$, i.e.,

$$Qf(x) = \lim_{t \to 0} \frac{1}{t} \left(\mathbb{E}_x f(X_t) - f(x) \right)$$

for $f \in \mathcal{D}(Q)$. The corresponding semigroup is denoted by S_t. For E compact S_t acts on $\mathcal{C}(E)$, the space of continuous functions, for cases such as $E = \mathbb{R}^d$, S_t acts on $\mathcal{C}_0(E)$, the space of continuous functions vanishing at infinity. We further denote $\mathcal{C}_b(E)$ the space of bounded continuous functions on E (of course in the compact case we have $\mathcal{C}(E) = \mathcal{C}_b(E)$). For μ a finite Borel measure on E and $f \in \mathcal{C}(E)$, we denote $\langle \mu, f \rangle = \int f d\mu$. We denote by $\mathcal{P}(E)$ the set of probability measures on E.

We now let $\{X_t^i : 0 \leq t \leq T\}$ be independent copies of the process $\{X_t : 0 \leq t \leq T\}$ starting at initial points $X_0^i = x_i$, and consider the empirical distribution

$$\mathcal{M}_N(t) = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_t^i} \tag{4.2.1}$$

This is a random probability measure on E, i.e., a random element of $\mathcal{P}(E)$, which in the limit $N \to \infty$ converges to the solution of the Kolmogorov forward equation.

If at time zero, $\mathcal{M}_N(0) \to \mu$ (where μ is a probability measure on E), then at time t, $\mathcal{M}_N(t) \to \mu_t$, where μ_t solves

$$\frac{d\mu_t}{dt} = Q^* \mu_t \tag{4.2.2}$$

where Q^* denotes the dual generator defined via

$$\langle \mu, Qf \rangle = \langle Q^* \mu, f \rangle$$

Indeed, by the law of large numbers, for all $f \in \mathcal{C}_b(E)$,

$$\langle \mathcal{M}_N(t), f \rangle = \sum_{i=1}^{N} \mathbb{E}_{x_i} f(X_t^i) \to \int f \, d\mu_t$$

where μ_t denotes the law of X_t when started initially from X_0 distributed according to μ.

The convergence $\mathcal{M}_N(t) \to \mu_t$ is a manifestation of the law of large numbers, and therefore it is natural to expect an associate large deviation principle, i.e.,

$$\mathbb{P}\left(\{\mathcal{M}_N(t) : 0 \leq t \leq T\} \approx \{\mu_t : 0 \leq t \leq T\} \right) \approx \exp\left(-N \mathcal{I}(\{\mu_t : 0 \leq t \leq T\}) \right) \tag{4.2.3}$$

where $\approx$ has to be interpreted in the sense of the large deviation principle, in a suitable topology on the space of trajectories. By the Markov property, the rate function $\mathcal{I}$ has the form of a Lagrangian "action"

$$\mathcal{I}\left(\{\mu_t : 0 \leq t \leq T\}\right) = \int_0^T \mathcal{L}(\mu_s, \dot{\mu}_s)\, ds \tag{4.2.4}$$

where $\dot{\mu}_s$ denotes the weak derivative of the trajectory at time s, defined via

$$\langle \dot{\mu}_s, f \rangle = \frac{d}{ds} \langle \mu_s, f \rangle$$

Our aim here is to compute the Lagrangian $\mathcal{L}$.

This opens the road to an analysis of bifurcation phenomena related to Gibbs-non-Gibbs transitions, as is done on the level of the magnetization in [9], [3]. The case of the empirical distribution would correspond to Gibbs-non-Gibbs phenomena in the context of mean-field models, where the mean field interaction is a function of possibly several empirical averages (rather than only of the magnetization).

Notice that the expression of $\mathcal{L}$ is independent of the precise topology (on the space of trajectories of probability measures on E) in which the large deviation principle (4.2.3) holds. As usual, one then first considers the weakest topology which is product topology (pointwise convergence at every time), and if one wants to strengthen the topology to e.g. uniform topology, one proves exponential tightness in that topology. In this paper we focus on the computation of the lagrangian $\mathcal{L}$ with the scheme of Feng and Kurtz [5], explained e.g. in [11].

In our context this means that we first compute the non-linear generator. To explain this, we need some more notation. First notice that $(X_t^1, X_t^2, \ldots, X_t^N)$ is a Markov process with generator

$$\mathcal{Q}_N f(x_1, \ldots, x_n) = \sum_{i=1}^N Q_i f \tag{4.2.5}$$

where Q_i denotes the generator Q applied to the i-th coordinate. Next, for N points $x_1, \ldots, x_N \in E$, and a function $F : \mathcal{P}(E) \to \mathbb{R}$ we use the notation $F(\mathcal{M}_N) = F\left(\frac{1}{N}\sum_{i=1}^N \delta_{x_i}\right)$.

The first computation in the Feng-Kurtz scheme is then the non-linear generator

$$HF(\mu) = \lim_{N\to\infty, \mathcal{M}_N(x_1,\ldots,x_n)\to\mu} \frac{1}{N}\left(e^{-NF(\mathcal{M}_N)}\mathcal{Q}_N e^{NF(\mathcal{M}_N)}\right) \tag{4.2.6}$$

If $\mathcal{H}F$ is of the form $\mathcal{H}(\mu, \nabla F)$, with $\mathcal{H}$ a strictly convex function in the second variable, then we call $\mathcal{H}(\mu, f)$ the Feng-Kurtz Hamiltonian, and the Lagrangian is then given by the Legendre transform of $\mathcal{H}$:

$$\mathcal{L}(\mu, \alpha) = \sup_{f\in\mathcal{C}(E)} \left(\int f\, d\alpha - \mathcal{H}(\mu, f)\right) \tag{4.2.7}$$

The interpretation of the "gradient" ∇F is straightforward when we are in the context of finite-state space Markov chains, because the set $\mathcal{P}(E)$ is then finite-dimensional. In the context of diffusion processes or more general Markov processes, the gradient will be a (context dependent) functional derivative.

The second variable of the Lagrangian (4.2.7) is the velocity variable, which in our context is a signed measure of total mass zero.

The Hamiltonian $\mathcal{H}(\mu, f)$ can then be obtained as follows:

$$\mathcal{H}(\mu, f) = \lim_{N\to\infty, \mathcal{M}_N \to \mu} \frac{1}{N} e^{-N\langle \mathcal{M}_N, f\rangle} \mathcal{Q}_N e^{N\langle \mathcal{M}_N, f\rangle} \tag{4.2.8}$$

Notice here that for a given $f \in \mathcal{C}(E)$, the function $e^{N\langle \mathcal{M}_N, f\rangle} = e^{\sum_{i=1}^N f(x_i)}$ is a function from E^N to $\mathbb{R}$, on which the generator $\mathcal{Q}_N$ can act, i.e., the notation in $\mathcal{Q}_N e^{N\langle \mathcal{M}_N, f\rangle}$ makes sense.

The μ variable is interpreted as the "position" and the f variable as the "momentum" (dual to the velocity variable in the Lagrangian formalism).

By the form (4.2.5) of the independent generator, the Hamiltonian can be computed:

$$\begin{aligned} \mathcal{H}(\mu, f) &= \lim_{N\to\infty, \mathcal{M}_N \to \mu} \frac{1}{N} e^{-N\langle \mathcal{M}_N, f\rangle} \mathcal{Q}_N e^{N\langle \mathcal{M}_N, f\rangle} \\ &= \lim_{N\to\infty, \mathcal{M}_N \to \mu} \frac{1}{N} \sum_{i=1}^N e^{-f(x_i)} Q e^{f(x_i)} \\ &= \int e^{-f} Q e^f \, d\mu \end{aligned} \tag{4.2.9}$$

Notice that since $\mathcal{H}(\mu, 0) = 0$, for the corresponding Lagrangian (4.2.7) we have

$$\mathcal{L}(\mu, \alpha) \geq (\langle \alpha, 0\rangle - \mathcal{H}(\mu, 0)) = 0$$

i.e., the Lagrangian is automatically non-negative (as it should be since it is the integrand of the rate function).

4.3 Finite-state space continuous-time Markov chains

In this case $E = \{a_1, \ldots, a_k\}$ is a finite set, of which we denote the elements by $a, b, \ldots$. The continuous-time Markov chain is defined via its transition rates between states $a, b \in E$, denoted by $r(a, b)$. The generator is given by

$$Qf(a) = \sum_{b\in E} r(a, b)(f(b) - f(a)) \tag{4.3.1}$$

and correspondingly, the Kolmogorov forward equation reads

$$\frac{d\mu_a(t)}{dt} = \sum_b (r(b,a)\mu_b(t) - r(a,b)\mu_a(t)) \tag{4.3.2}$$

Since a function $f : E \to \mathbb{R}$ is identified with a column of numbers $f_a, a \in E$, we will use both notations $f(a)$, or f_a, idem for probability measures (identified with rows $\mu_a, a \in E$). The Hamiltonian (4.2.9) is given by

$$\mathcal{H}(\mu, f) = \sum_{a,b\in E} \mu_a r(a,b)(e^{f_b - f_a} - 1) \tag{4.3.3}$$

The Lagrangian is then

$$\mathcal{L}(\mu, \alpha) = \sup_f \left(\sum_a f_a \alpha_a - \mathcal{H}(\mu, f) \right) \tag{4.3.4}$$

The $f = f^*(\alpha)$ which realizes the supremum satisfies

$$\alpha_b = \sum_a \left(\mu_a r(a,b) e^{f_b^* - f_a^*} - \mu_b r(b,a) e^{f_a^* - f_b^*} \right) \tag{4.3.5}$$

which then gives

$$L(\mu, \alpha) = \sum_{a,b} \mu_b r(b,a) \left(f_a^* e^{f_a^* - f_b^*} - f_b^* e^{f_a^* - f_b^*} - (e^{f_a^* - f_b^*} - 1) \right) \tag{4.3.6}$$

defining the "modified" rates

$$r^*(b,a) = r(b,a) e^{f_a^* - f_b^*}$$

the equation (4.3.5) reads

$$\alpha_b = \sum_a (\mu_a r^*(a,b) - \mu_b r^*(b,a)) \tag{4.3.7}$$

which can be interpreted as follows. The modified rates are such that they produce "velocity" ((4.3.2)) equal to α, when started from initial measure μ. In terms of these modified rates r^*, the Lagrangian reads

$$L(\mu, \alpha) = \sum_{a,b} \mu_b r^*(b,a) \log \left(\frac{r^*(b,a)}{r(b,a)} \right) - \sum_{a,b} \mu_b (r^*(b,a) - r(b,a)) \tag{4.3.8}$$

This can be interpreted in terms of relative entropy as follows. The Radon-Nikodym derivative of the path space measure of the process with rates r^* w.r.t. the process with rates r is given by the Girsanov formula

$$\frac{d\mathbb{P}_{r^*}^{[0,T]}}{d\mathbb{P}_r^{[0,T]}}(\omega) = \exp \left(\sum_{a,b} \left(\log \left(\frac{r^*(b,a)}{r(b,a)} \right) N_T^{b,a} - (r^*(b,a) - r(b,a)) l(T,b,\omega) \right) \right) \tag{4.3.9}$$

where $N_t^{(b,a)}$ denotes the number of transitions from b to a in $[0,t]$ and where $l(T,b,\omega)$ denotes the total time that the path ω spends in state b. The corresponding relative entropy is

$$s(\mathbb{P}_{r^*}^{[0,T]}|\mathbb{P}_r^{[0,T]}) = \int d\mathbb{P}_{r^*}^{[0,T]} \log\left(\frac{d\mathbb{P}_{r^*}^{[0,T]}}{d\mathbb{P}_r^{[0,T]}}\right)$$

Taking the limit $T \to 0$ in this expression, starting from initial distribution μ, we find

$$\lim_{T\to 0} \frac{1}{T} s(\mathbb{P}_{r^*}^{[0,T]}|\mathbb{P}_r^{[0,T]}) = \mathcal{L}(\mu,\alpha) \tag{4.3.10}$$

In words this means the following. In order to compute $\mathcal{L}(\mu,\alpha)$, we have to consider an auxiliary Markov process with rates that from starting from μ produce velocity (in the sense of (4.3.2)) equal to α. The relative entropy of this process w.r.t. the original process in a small interval of time $[0,t]$ is then given by $t\mathcal{L}(\mu,\alpha) + O(t^2)$. The Lagrangian $\mathcal{L}(\mu,\alpha)$ can thus be viewed as a "relative entropy production" needed to force the process to have speed α when started from μ. In particular for $\alpha = Q^*\mu$, the cost is zero, and we have $\mathcal{L}(\mu, Q^*\mu) = 0$. This shows that the evolution according to the Kolmogorov forward equation is of course an optimal trajectory, with zero cost.

4.3.1 Hamiltonian trajectories for finite Markov chains

The Hamiltonian (4.3.3) has Hamiltonian trajectories given by

$$\begin{aligned} \dot{f}_a &= -\frac{\partial \mathcal{H}}{\partial \mu_a} = -\sum_b r(a,b)(e^{f_a - f_b} - 1) \\ \dot{\mu}_a &= \frac{\partial \mathcal{H}}{\partial f_a} = \sum_b \left(\mu_b r(b,a) e^{f_a - f_b} - \mu_a r(a,b) e^{f_b - f_a}\right) \end{aligned} \tag{4.3.11}$$

The interpretation of the second equation is the following. For a trajectory with "momentum" f, the motion of the probability measure is that of a Markov process with rates which are modified according to f via

$$\tilde{r}(a,b) = r(a,b) e^{f_b - f_a} \tag{4.3.12}$$

Indeed, for the modified rates $\tilde{r}$, the second equation of (4.3.11) reads simply

$$\dot{\mu}_a = \sum_b \mu_b \tilde{r}(b,a) - \mu_a \tilde{r}(a,b)$$

which is precisely the Kolomogorov forward equation for the evolution of a probability distribution in a Markov chain with rates $\tilde{r}$.

The equation for the momenta, i.e., the first equation of (4.3.11) can be rewritten using the variables $u_a = e^{f_a}, a \in E$:

$$\dot{u}_a = -\sum_b r(a,b)(u_b - u_a) = -(Qu)_a$$

which has the solution

$$u(t) = e^{-tQ}u(0) \tag{4.3.13}$$

The equation for the "position variables " μ_a is linear and reads

$$\mu(t) = M(u(t))\mu(t) \tag{4.3.14}$$

with M a matrix depending on the solution of the momentum variables, given by

$$M_{a,b}(f) = r(b,a)\frac{u_a}{u_b} - \left(\sum_c r(a,c)\frac{u_c}{u_a}\right)\delta_{a,b} \tag{4.3.15}$$

This matrix has column sums equal to zero, i.e., for all $b \in E$ we have $\sum_a M_{a,b} = 0$, which corresponds to the conservation of mass $\sum_a \mu_a(t) = 1$ in the Hamiltonian evolution. More precisely, the matrix $M_{a,b}$ is precisely the adjoint of the generator corresponding to the modified rates $\tilde{r}$ defined in (4.3.12).

We thus conclude that the Hamiltonian trajectories are still Markovian, corresponding with time-dependendent rates, steered by the solution of the momentum equation (4.3.13).

The solution of (4.3.14) is given by

$$\mu(t) = e^{\int_0^t M(u(s))}\mu(0) \tag{4.3.16}$$

which means that we have the form of the optimal trajectories, with integration constants given by $u(0)$ and $\mu(0)$. Although the form (4.3.16), (4.3.13) looks quite explicit, it is not easy in general to find explicit tractable formulas for $\mu(t)$. The action or path-space cost

$$\mathcal{I} = \int_0^T \mathcal{L}(\mu_s, \dot{\mu}_s)\ ds$$

can be rewritten in Hamiltonian formalism as

$$\mathcal{J}(\{\mu(s), f(s) : 0 \le s \le T\}) = \sum_a \int_0^T f_a(t)\dot{\mu}_a(t)\ dt - \mathcal{H}(\mu(0), f(0)) \tag{4.3.17}$$

This means that in order to find the optimal cost between a measure $\mu(0) = \mu$ and a measure $\mu(T) = \nu$ at time T, one has to plug in the solution (4.3.16), (4.3.14) into the expression (4.3.17), and determine the integration constants $\mu(0), f(0)$ by initial and final condition. This leads to a function $\Psi(\mu, \nu, T)$ which is the optimal path cost to travel from μ to ν in time T. In concrete situations beyond two-state Markov chains, in practice, this function is hard to obtain closed formulas for (an issue which we do not want to pursue here).

4.3.1.1 Two-state symmetric flipping

To see an example of an explicit solution, we consider the case of two-states flipping at rate 1, which corresponds with mean-field independent spin flip dynamics, treated before in [9], [3], [11].

In that case, the state space is given by $E = \{1, 2\}$, the matrix Q is given by

$$Q = \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}$$

and the matrix M of (4.3.15) is given by

$$M = \begin{pmatrix} -\frac{u_2}{u_1} & \frac{u_1}{u_2} \\ \frac{u_2}{u_1} & -\frac{u_1}{u_2} \end{pmatrix}$$

where $u = (u_1, u_2)^T$ satisfies

$$\dot{u} = -Qu \tag{4.3.18}$$

The equation

$$\dot{\mu} = M\mu$$

can be differentiated w.r.t. time once more, which gives

$$\frac{d^2\mu}{dt^2} = \left(\frac{dM}{dt} + M^2\right)\mu$$

Explicit computation, using (4.3.18) then gives

$$\frac{dM}{dt} + M^2 = \begin{pmatrix} 2 & -2 \\ -2 & 2 \end{pmatrix}$$

which gives the equations

$$\frac{d^2\mu_1(t)}{dt^2} = 2\mu_1(t) - 2\mu_2(t) = -2\frac{d^2\mu_2(t)}{dt^2}$$

Putting $\mu_1 - \mu_2 = x$ we have,

$$\frac{d^2x}{dt^2} = 4x$$

which gives $x_t = C_1e^{2t} + C_2e^{-2t}$ as optimal solutions, consistent with e.g. [9], or [3].

Remark 4. *The fact that $\frac{dM}{dt} + M^2$ is a constant matrix is quite exceptional. Even in the two-state case, if the rates $r(1,2) = \alpha \neq r(2,1) = \beta$, the matrix $\frac{dM}{dt} + M^2$ is not constant and differentiating the equation* (4.3.14) *once more does not lead to further simplification.*

4.4 Diffusion processes

Here we consider the state space $E = \mathbb{R}^n$ and diffusion processes with generator

$$Q = \sum_i b_i(x)\partial_i + \sum_{ij} a_{ij}(x)\partial_{ij}^2 \tag{4.4.1}$$

where ∂_i denotes partial derivative w.r.t. x_i. Here $b_i(x)$, $a_{ij}(x)$ are supposed to be Lipschitz and sufficiently smooth, ensuring the existence of a solution of the martingale problem associated to Q.

The covariance $a_{ij}(x)$ is supposed to be a positive definite matrix. Moreover, for simplicity we assume that it is bounded from below by a multiple of the identity (to avoid degeneracies).

The Feng-Kurtz Hamiltonian $\mathcal{H}(\mu, f)$ ((4.2.9)) can then be computed and this yields:

$$\begin{aligned} \mathcal{H}(\mu, f) &= e^{-f} Q e^{f} \, d\mu \\ &= \int \left(Qf + \sum_{ij} \partial_i f(x) \partial_j f(x) a_{ij}(x) \right) \, d\mu(x) \end{aligned} \tag{4.4.2}$$

The measures μ that we will have to consider are absolutely continuous probability measures w.r.t. Lebesgue measure, $\mu = \mu(x)dx$, where with slight abuse of notation we use the symbol μ both for the measure and for the density.

Although we are in the infinite-dimensional context here, since the Hamiltonian is quadratic, the corresponding Lagrangian can be obtained more easily than in the previous subsection.

Define the quadratic form

$$J_\mu(f, f) = \int \left(\sum_{ij} \partial_i f(x) \partial_j f(x) a_{ij}(x) \right) \, d\mu(x) \tag{4.4.3}$$

To this quadratic form corresponds a positive self-adjoint operator A_μ (linearly depending on μ) such that

$$J_\mu(f, f) = \frac{1}{2} \langle f, A_\mu f \rangle$$

where $\langle f, g \rangle = \int f(x) g(x) \, dx$ is the usual L^2 innerproduct.

With this notation, the Hamiltonian can be written in the form

$$\mathcal{H}(\mu, f) = \langle \mu, Qf \rangle + \frac{1}{2} \langle f, A_\mu f \rangle = \langle Q^* \mu, f \rangle + \frac{1}{2} \langle f, A_\mu f \rangle \tag{4.4.4}$$

Then, the corresponding Lagrangian is computed

$$\begin{aligned}\mathcal{L}(\mu,\alpha) &= \sup_f \left(\langle f, \alpha\rangle - \langle Q^*\mu, f\rangle - \frac{1}{2}\langle f, A_\mu f\rangle \right) \\ &= \frac{1}{2}\langle (\alpha - Q^*\mu), A_\mu^{-1}(\alpha - Q^*\mu)\rangle \end{aligned} \tag{4.4.5}$$

The rigorous meaning of $\langle f, A_\mu^{-1} f\rangle$ is $\|A_\mu^{-1/2} f\|_2^2$ for f in the domain of $A_\mu^{-1/2}$. The Lagrangian is then defined to be infinite when $(\alpha - Q^*\mu)$ is not in the domain of $A_\mu^{-1/2}$ (cf. the abstract form of Schilder's theorem in abstract Wiener spaces see [1]).

We see that the "typical trajectory" which follows the Kolmogorov forward equation has zero cost, since in that case $\dot\mu = \alpha = Q^*\mu$, and hence $\mathcal{L}(\mu,\alpha) = 0$, and the Lagrangian is a quadratic expression in the deviation of the trajectory from the Kolmogorov forward equation.

To illustrate this formula, let us consider first the simplest example of the present context, i.e., dimension $n = 1$, drift $b = 0$, $a = 1/2$, corresponding to a one-dimensional Brownian motion. The generator is

$$Q = \frac{1}{2}\frac{d^2}{dx^2}$$

$Q^* = Q$. The quadratic form (4.4.3) reads in this case

$$J_\mu(f,f) = \frac{1}{2}\int \mu(x)(f')^2 dx$$

and the corresponding operator

$$A_\mu = \frac{d}{dx}\left(\mu(x)\frac{d}{dx}\right)$$

which gives

$$\mathcal{L}(\mu,\alpha) = \frac{1}{2}\left\langle \nabla^{-1}\left(\alpha - \frac{1}{2}\mu''\right), \frac{1}{\mu}\nabla^{-1}\left(\alpha - \frac{1}{2}\mu''\right)\right\rangle \tag{4.4.6}$$

The rigorous meaning of the formal expression $\langle \nabla^{-1} f, \nabla^{-1} g\rangle$ is the innerproduct in the space H^{-1}, i.e., $\langle (-\Delta)^{-1/2} f, (-\Delta)^{-1/2} g\rangle$, with $\Delta = \frac{d^2}{dx^2}$, the Laplacian.

Remark 5. *The rate function* (4.4.6) *has also been obtained in the context of the study of the hydrodynamic limit for independent Brownian particles, in [8]. In general, it is an interesting question to understand the relation between the rate functions which are computed in this paper and the rate functions for deviations of the hydrodynamic limit, see e.g. [7]. For Brownian particles, they coincide because of scale invariance of the Brownian motion.*

The Lagrangian (4.4.6) can be interpreted in terms of relative entropy. A diffusion process on $\mathbb{R}$ with drift $b(x)$ and variance equal to one has the generator

$$Q_b = b(x)\frac{d}{dx} + \frac{1}{2}\frac{d^2}{dx^2}$$

if we start this process from a measure $\mu = \mu(x)dx$, then the infinitesimal change at time zero is given by the adjoint generator working on μ, i.e.,

$$\frac{1}{2}\frac{d^2\mu(x)}{dx^2} + \frac{d}{dx}(b(x)\mu(x)) = (Q_b^*\mu)(x) \tag{4.4.8}$$

In particular, for α, a given absolutely continuous signed measure of total mass zero, we can find the drift b that corresponds to it, i.e., solving the equation

$$\frac{1}{2}\frac{d^2\mu(x)}{dx^2} + \frac{d}{dx}(b(x)\mu(x)) = \alpha(x) \tag{4.4.9}$$

The process with drift b has a corresponding path space measure on Wiener space given by $\mathbb{P}_b^{[0,T]}$, and we have the Girsanov formula

$$\frac{d\mathbb{P}_b}{d\mathbb{P}_0} = \exp\left(\int_0^T b(W_s)dW_s - \frac{1}{2}\int_0^T b^2(W_s)ds\right) \tag{4.4.10}$$

The relative entropy of the process with drift b w.r.t. the zero drift process is thus given by

$$\begin{aligned} & s(\mathbb{P}_b^{[0,T]}|\mathbb{P}_0^{[0,T]}) = \int d\mathbb{P}_b \log\left(\frac{d\mathbb{P}_b}{d\mathbb{P}_0}\right) \\ = \;& \mathbb{E}_0\left(\left(\int_0^T b(W_s)dW_s - \frac{1}{2}\int_0^T b^2(W_s)ds\right)\exp\left(\int_0^T b(W_s)dW_s - \frac{1}{2}\int_0^T b^2(W_s)ds\right)\right) \end{aligned} \tag{4.4.11}$$

where the expectation $\mathbb{E}_0$ is over the standard Brownian motion. Computing then

$$\lim_{T\to 0}\frac{1}{T}s(\mathbb{P}_b^{[0,T]}|\mathbb{P}_0^{[0,T]})$$

using a starting distribution μ gives exactly the expression

$$\frac{1}{2}\int b^2(x)\mu(x)dx$$

which equals $\mathcal{L}(\mu,\alpha)$ of (4.4.6), because by (4.4.9)

$$\frac{d}{dx}(b(x)\mu(x)) = \alpha - \frac{1}{2}\mu''(x)$$

Hence, as in the finite Markov chain case, we see that the Lagrangian can be interpreted as the infinitesimal relative entropy cost to produce a derivative measure α when started from μ. In particular, when $\alpha = Q^*\mu$ this cost is zero, showing once more (in this context) that the evolution according to the Kolmogorov forward equation is an optimal trajectory with zero cost.

4.5 Trajectory of the empirical measure

4.5.1 Context and notation

In the context of translation invariant interacting systems, the empirical distribution is no longer a natural object because of interactions. The natural object capturing the essential information about the time evolution, modulo translations is the empirical measure. In order to describe this context, we need some more notation. For $N \in \mathbb{N}$ we denote $V_N = \{-N, \dots, N\}^d$ and denote by $\mathbb{T}_d^N$ the d-dimensional torus, i.e., V_N endowed with addition modulo $2N+1$.

We will consider translation invariant systems on this torus which for large N have to be thought of as approximations of an infinite interacting system where the individual components live on the lattice $\mathbb{Z}^d$.

The configuration space is $\Omega_N = E^{\mathbb{T}_d^N}$, where E, the single-site space, is a locally compact Polish space. Further we denote $\Omega = E^{\mathbb{Z}^d}$ As in the previous sections, we mostly consider E or a finite set (interacting particle systems) or E a submanifold of $\mathbb{R}^n$ (diffusion processes). Elements of Ω_N are denoted $\sigma, \eta, \xi, \dots$, and for $\sigma \in \Omega_N$, $i \in \mathbb{T}_{d\ N}^N$, σ_i denotes the value of the configuration at site i. On $\mathbb{T}_{d\ N}^N$ we have the addition modulo N, and correspondingly, the shift τ_i defined on Ω_N via

$$(\tau_i(\sigma))_j = \sigma_{j+i} \tag{4.5.1}$$

on functions $f : \Omega_N \to \mathbb{R}$ via $\tau_i f(\sigma) = f(\tau_i \sigma)$, and on probability measures via $\int f d(\tau_i \mu) = \int \tau_i f d\mu$. If A is a linear operator on functions $f : \Omega_N \to \mathbb{R}$ then we define its shift over i to be $\tau_i A \tau_{-i}$, and an operator is called translation invariant if for all i, $\tau_i A \tau_{-i} = Q$. A measure is translation invariant if $\tau_i \mu = \mu$. Natural translation invariant measures on Ω_N are obtained by periodizing translation invariant measures on Ω, i.e., starting from σ distributed according to a translation invariant measure on Ω, we consider $\sigma_i^N = \sigma_i, i \in V_N$, periodically extended to the whole lattice. Conversely, if we have a probability measure on Ω_N we naturally associate to it a probability measure on the infinite configuration space Ω. This justifies the fact that with slight abuse of notation we can use sometimes the same symbol μ_N for a translation invariant measure on Ω_N as well as for a translation invariant measure on Ω. We denote by $\mathbb{P}_{inv}(\Omega)$ the set of translation invariant probability measures on Ω.

A function $f : \Omega \to \mathbb{R}$ is called local if it depends on a finite number of coordinates, i.e., if there exists a (minimal) finite set D_f, called the dependence set of f such that for all $\sigma, \eta \in \Omega$: $f(\sigma_{D_f} \eta_{\mathbb{Z}^d \setminus D_f}) = f(\sigma)$, i.e., the value of the function is not influenced

by changing the configuration outside D_f. Obviously, a local function $f : \Omega \to \mathbb{R}$ can be thought of as being a function $f : \Omega_N \to \mathbb{R}$ as well, for N large enough such that $V_N \supset D_f$. The translation $\tau_i f$ of local function is obviously local, with dependence set $D_{\tau_i f} = D_f + i = \{x + i : x \in D_f\}$.

An linear operator (possibly unbounded) $A : \mathcal{D}(A) \subseteq \mathcal{C}(\Omega) \to \mathcal{C}(\Omega)$ is local if it acts only on a finite set of coordinates. As for a local function, a local operator acts naturally on functions $f : \Omega_N \to \mathbb{R}$ for N large enough.

4.5.2 Translation invariant sequence of local generators

Definition 2. *A translation invariant sequence of local generators is defined to be a a sequence of generators of the form $\mathcal{L}_N = \sum_{i \in \mathbb{T}_d^N} \tau_i Q \tau_{-i}$, with Q a local generator, such that the corresponding infinite-volume generator $\mathcal{L} = \sum_{i \in \mathbb{Z}^d} \tau_i Q \tau_{-i}$ is well-defined and has a core consisting of local functions as a core. The generator Q is called the "source generator".*

Remark 6. *For E discrete, the core in Definition 2 consists typically of all local functions, whereas for E being an interval or non-discrete, typically the core consists of smooth local functions.*

As a consequence, the corresponding processes $\{\sigma_{N,t} : t \geq 0\}$ converge weakly in path space to the infinite-volume process $\{\sigma_t : 0 \leq t \leq T\}$ with generator $\mathcal{L}$. Moreover, for the associated semigroups we have that $S_t^N f \to S_t f$ uniformly as $N \to \infty$, for all local functions f.

Let us give sone examples in order to make this concept more concrete.

1. **Independent Markov processes.** For Q a generator of a Markov process on E, we define
$$\mathcal{L}_N = \sum_{i \in \mathbb{T}_d^N} \tau_i Q \tau_{-i}$$
Under the process with generator $\mathcal{L}_N$ different components evolve independently, as copies of the process with generator Q.

2. **Spin-flip dynamics.** E is finite set (e.g. $E = \{-1, 1\}$ for Ising spins), $\theta : E \to E$ a bijection such that $\theta(a) \neq a$ for all $a \in E$. Furthermore, a local function $r : \Omega \to \mathbb{R}^+$, with dependence set containing the origin, is given. The local generator is then defined $Qf(\sigma) = r(\sigma) f(\theta_0 \sigma) - f(\sigma)$, where θ_0 means applying θ to the coordinate σ_0 and leaving all other coordinates unchanged (similarly we denote θ_i). The corresponding sequence of generators is then given by
$$\mathcal{L}_N f(\sigma) = \sum_i ((\tau_i Q \tau_{-i}) f)(\sigma) = \sum_{i \in \mathbb{T}_d^N} r(\tau_i \sigma)(f(\theta_i \sigma) - f(\sigma))$$

3. **Interacting diffusions.** For $E = \mathbb{R}$ and for a finite set $D \subseteq \mathbb{Z}^d$, we consider the local generator

$$Qf(\sigma) = \left(\sum_{i \in D} \frac{\partial V(\sigma_D)}{\partial \sigma_0} \frac{\partial}{\partial \sigma_i} \right) + \frac{1}{2} \frac{\partial^2}{\partial \sigma_0^2}$$

and the corresponding

$$\mathcal{L}_N = \sum_i \tau_i Q \tau_{-i} f$$

This represents a system of diffusions, interacting via the potential V. E.g. for a nearest neighbor potential $V : \mathbb{R} \to \mathbb{R}$ in $d = 1$, the full generator has the form

$$\sum_i V'(|\sigma_i - \sigma_{i-1}|) \left(\frac{\partial}{\partial \sigma_i} - \frac{\partial}{\partial \sigma_{i-1}} \right) + \frac{1}{2} \frac{\partial^2}{\partial \sigma_i^2}$$

corresponding to $D = \{0, 1\}$, $V(\sigma_D) = V(|\sigma_1 - \sigma_0|)$.

4. **Local interacting particle systems.** E is a finite set. For finite subsets $D_\alpha \subseteq \mathbb{Z}^d$, a collection of $T_\alpha : E^{D_\alpha} \to E^{D_\alpha}$ $\alpha \in \{1, \ldots, k\}$, and corresponding rates $c(\alpha, \sigma)$ we consider the local generator

$$Qf(\sigma) = \sum_\alpha c(\alpha, \sigma)(f(T_\alpha \sigma_{D_\alpha} \sigma_{D_\alpha^c}) - f(\sigma))$$

the corresponding local generators then include of course the previous spin-flip case but also translation invariant spin-exchange (Kawasaki) dynamics, combination of spin-flip and spin-exchange, etc.

5. **Local averaging.** For $0 \in D \subseteq \mathbb{Z}^d$ finite, and m_D a probability measure on A^D, consider

$$Qf(\sigma) = r(\sigma) \int \left(f(\sigma'_D \sigma_{D^c}) - f(\sigma) \right) m_D(d\sigma'_D)$$

with r a local function. In words, this means that with rate r, the configuration inside D is replaced by its average over the measure m_D. An important example of this class is the KMP model of heat conduction.

4.5.3 Trajectory of the empirical measure

For a configuration $\sigma \in \Omega_N$, its empirical measure is defined by

$$\mathbb{L}_N(\sigma) = \frac{1}{|\mathbb{T}_d^N|} \sum_{i \in \mathbb{T}_d^N} \delta_{\tau_i \sigma} \tag{4.5.4}$$

this is a translation invariant probability measure on Ω_N, capturing all information about σ, modulo translations.

For a configuration on the full lattice, $\sigma \in \Omega$, with a slight abuse of notation we also denote

$$\mathbb{L}_N(\sigma) = \frac{1}{|\mathbb{T}_d^N|} \sum_{i \in \mathbb{T}_d^N} \delta_{\tau_i(\sigma^N)} \tag{4.5.5}$$

where σ^N is the periodized configuration obtained from σ.

If μ is a probability measure on Ω, which is ergodic under translations, then, by the Birkhoff ergodic theorem, with μ probability one

$$\mathbb{L}_N(\sigma) \to \mu$$

as $N \to \infty$, where $\to$ means weak convergence.

If $(\mathcal{L}_N)_N$ is a translation invariant sequence of local generators, then we have the associated Markov processes $\sigma_{N,t}$ with semigroups $S_t^N = e^{t\mathcal{L}_N}$. For a probability measure μ on Ω, let us denote μ_t to be the distribution at time $t > 0$ in the infinite-volume process $\{\sigma_t : t \geq 0\}$, started at initial state distributed according to μ. By locality of the generator $\mathcal{L}$, for μ ergodic, we have that μ_t is ergodic as well and hence

$$\mathbb{L}_N(\sigma_t) \to \mu_t$$

weakly, with probability one. Hence the random trajectory of translation invariant probability measures $\{\mathbb{L}_N(\sigma_t) : 0 \leq t \leq T\}$ converges, as $N \to \infty$ to the deterministic trajectory $\{\mu_t : 0 \leq t \leq T\}$. This convergence of a random $\mathcal{P}_{inv}(\Omega)$-valued trajectory to a deterministic $\mathcal{P}_{inv}(\Omega)$-valued trajectory can be thought of as a law of large numbers (in an infinite-dimensional space), and therefore it is natural to ask for an associated large deviation principle. For spin-flip dynamics, this was studied in [3]. Here we treat the general case of a translation invariant sequence of local generators. This will naturally lead to a non-linear operator $\mathcal{K}_Q$ associated to the local generator Q, which will be the analogue in the present context of the non-linear operator $e^{-f}Qe^f$ in the previous section.

More precisely, we want to identify the "path space Lagrangian" (which is in this section is denoted by Ξ) such that

$$\mathbb{P}\left(\{\mathbb{L}_N(\sigma_t) : 0 \leq t \leq T\} \approx \{\nu_t : 0 \leq t \leq T\}\right) \approx \exp\left(-|\mathbb{T}_d^N| \int_0^T \Xi(\nu_t, \dot{\nu}_t)\right)$$

The Lagrangian is now a function of a translation invariant probability measure and a translation invariant signed measure of total mass zero, and as before, $\approx$ has to be interpreted in the sense of the large deviation principle, in this case, in the space of trajectories of translation invariant measures.

4.5.4 The Feng-Kurtz Hamiltonian

In this section we compute the Feng-Kurtz Hamiltonian. This Hamiltonian is now a function from $\mathcal{C}(\Omega) \times \mathcal{P}_{inv}(\Omega)$ to $\mathbb{R}$, where the first variable has to be thought of as the "position" variable, whereas the second variable functions as a momentum variable. The Hamiltonian is defined as the limit

$$\mathcal{H}(\mu, f) = \lim_{N\to\infty, \mathcal{L}_N(\sigma)\to\mu} \frac{1}{|\mathbb{T}_d^N|} \left(e^{-|\mathbb{T}_d^N|\langle \mathbb{L}_N(\sigma), f\rangle} \mathcal{L}_N e^{|\mathbb{T}_d^N|\langle \mathbb{L}_N(\sigma), f\rangle} \right) \tag{4.5.6}$$

Note that $|\mathbb{T}_d^N|\langle \mathbb{L}_N(\sigma), f\rangle = \sum_{i\in\mathbb{T}_d^N} \tau_i f(\sigma)$.

For the computation of (4.5.6), we assume f to be a local function. Because the source generator Q is local we have, that $Q(\tau_k f) = 0$ for all k outside the set $D(Q, f) = \{k : D_Q \cap D_f + k \neq \varnothing\}$. Therefore, for $\Lambda \subseteq \mathbb{Z}^d$ finite,

$$Q\left(\prod_{i\in\Lambda} \tau_i f\right) = \left(\prod_{i\in\Lambda\setminus D(Q,f)} \tau_i f\right) Q\left(\prod_{i\in\Lambda\cap D(Q,f)} \tau_i f\right) \tag{4.5.7}$$

Use (4.5.7) to compute

$$\begin{aligned}
\mathcal{H}(\mu, f) &= \lim e^{-\sum_i \tau_i f} \sum_j \tau_j \left(Q e^{\sum_i \tau_{i-j} f} \right) \\
&= e^{\sum_i \tau_i f} \sum_j \tau_j \left(Q e^{\sum_{i\in D(f,Q)+j} \tau_{i-j} f} \right) e^{\sum_{i\notin D(f,Q)+j} \tau_i f} \\
&= \sum_j \tau_j \left(e^{-\sum_{i\in D(f,Q)+j} \tau_{i-j} f} Q e^{\sum_{i\in D(f,Q)+j} \tau_{i-j} f} \right) \\
&= \sum_j \tau_j \left(e^{-\sum_{k\in D(f,Q)} \tau_k f} Q e^{\sum_{k\in D(f,Q)} \tau_k f} \right)
\end{aligned} \tag{4.5.8}$$

We can now introduce the non-linear operator associated to the "source" generator Q, working on local functions f:

$$\mathcal{K}_Q f = e^{-\sum_{k\in D(f,Q)} \tau_k f} Q e^{\sum_{k\in D(f,Q)} \tau_k f} \tag{4.5.9}$$

Using this notation, we obtain from (4.5.8)

$$\mathcal{H}(\mu, f) = \int \mathcal{K}_Q(f) d\mu \tag{4.5.10}$$

This Hamiltonian has to be thought of as the analogue of (4.2.9) in the present context.

Remark 7. *Note that we can write, informally,*

$$\mathcal{K}_Q f = e^{-\sum_{k\in\mathbb{Z}^d} \tau_k f} Q e^{\sum_{k\in\mathbb{Z}^d} \tau_k f}$$

since the terms $k \notin D(f,Q)$ "cancel". This is of course not rigorous because the sum $\sum_{k\in\mathbb{Z}^d} \tau_k f$ is divergent, but this divergence is the "same" as for a formal infinite-volume Hamiltonian, where energy differences are well defined. The advantage of this formal representation is that we clearly see that $\mathcal{K}$ is a translation invariant operator, i.e., $\mathcal{K}_Q(f) = \mathcal{K}_Q(\tau_i f)$, and as a consequence, the Hamiltonian $\mathcal{H}(\mu, f)$ is translation invariant as well, both in the measure and in the function, i.e.,

$$\mathcal{H}(\tau_k\mu, \tau_r f) = \mathcal{H}(\mu, f)$$

for all $k, r \in \mathbb{Z}^d$. Another advantage is that one clearly sees the analogy with the corresponding formula for the empirical distribution (4.2.9).

The corresponding Lagrangian is then found by Legendre transformation, i.e.,

$$\Xi(\mu, \dot\mu) = \sup_{f\in\mathcal{C}(\Omega)} \left(\int f d\dot\mu - \mathcal{H}(\mu, f) \right) \tag{4.5.12}$$

where $\dot\mu$ denotes a translation invariant signed measure of total mass zero, and μ a translation invariant probability measure on Ω.

In general, an explicit expression for Ξ cannot be obtained easily. In the examples below we will compute Ξ quite explicitly for diffusion processes and show a relative entropy interpretation of Ξ both in the context of interacting particle systems (analogue of finite Markov chains in the previous section) and in the context of interacting diffusions.

4.5.5 Interacting particle systems

We now compute $\mathcal{K}_Q$ for some of the examples discussed before, starting with interacting particle systems. The local generator is of the form.

$$Qf = \sum_\alpha r_\alpha (T_\alpha f - f)$$

where T_α are local transformations, which change coordinates only in a finite set D_α containing the origin. This gives

$$\mathcal{K}_Q f = \sum_\alpha r_\alpha \left(e^{\mathcal{D}_\alpha(f)} - 1 \right) \tag{4.5.13}$$

where the operator $\mathcal{D}_\alpha$ is defined by

$$\mathcal{D}_\alpha f = \sum_{k\in\mathbb{Z}^d} (T_\alpha(\tau_k f) - \tau_k f)$$

Notice that the sum is in fact a finite sum since f is local, and the transformation T_α is local as well. Let us now zoom in into two familiar examples.

- **Independent spin-flip**. For $E = \{-1, 1\}$, and for a single transformation $T\sigma = \sigma^0$ (spin-flip), we get

$$\mathcal{D}(f) = \sum_{k \in -D_f} (\tau_k f(\sigma^0) - \tau_k f)$$

for the special functions $f(\sigma) = H_A(\sigma) = \prod_{i \in A} \sigma_i$ we get

$$\mathcal{D}(H_A) = \sum_{k \in -A} -2H_{A+k}$$

as we found before in [3].

- **Exclusion process**. For $E = \{0, 1\}$, $d = 1$ and $T(\sigma) = \sigma^{01}$, where σ^{01} denotes exchange of the values at site 0 and 1, i.e., $(\sigma^{01})_j = \sigma_1\delta_{j,0} + \sigma_0\delta_{j,1} + \sigma_j(1 - \delta_{j,0} - \delta_{j,1})$. We have

$$\mathcal{D}(f)(\eta) = \sum_{k : k + D_f \cap \{0,1\} \neq \varnothing} f(\tau^k(\eta^{01})) - f(\eta)$$

Notice that for $f = \eta_j$ we find only two terms contributing to $\mathcal{D}(f)$:

$$\begin{aligned} \mathcal{D}(f) &= \left((\tau^{-j}(\eta^{01}))_j - (\tau^{-j}(\eta))_j\right) + \left((\tau^{-j+1}(\eta^{01}))_j - (\tau^{-j+1}(\eta))_j\right) \\ &= \eta_1 - \eta_0 + \eta_0 - \eta_1 = 0 \end{aligned}$$

which corresponds to the fact that the density of particles is conserved in this process.

The Lagrangian associated with (4.5.13) is

$$\Xi(\mu, \dot{\mu}) = \sup_{f \in \mathcal{C}(\Omega)} \left(\int f d\dot{\mu} - \int \left(\sum_\alpha r_\alpha \left(e^{\mathcal{D}_\alpha(f)} - 1 \right) \right) d\mu \right) \tag{4.5.14}$$

This expression is reminiscent of (4.3.4) in section 3 (empirical distribution for finite Markov chains). Indeed, a similar relative entropy interpretation of this expression can be given. We will describe this rather informally, making the arguments rigorous here is however completely standard and analogous to the Girsanov formula computation of the section on finite Markov chains. First we not that for a translation invariant measure μ, its "derivative at time zero" $\mathcal{L}^*\mu$ is formally given by

$$(\mathcal{L}^*\mu)(\sigma) = \sum_i \sum_\alpha (r_\alpha(\tau_i\sigma)\mu(\tau_i T_\alpha \tau_{-i}\sigma) - r_\alpha(\tau_i\sigma)\mu(\tau_i\sigma))$$

Suppose now we consider modified rates $\tilde{r}_\alpha(\sigma) = r_\alpha(\sigma)e^{f(\sigma) - f(T_\alpha(\sigma))}$, and the associated modified local generator $\tilde{Q} = \sum_\alpha \tilde{r}_\alpha(T_\alpha - I)$, i.e., the same transformations are applied with other rates. Then for a given translation invariant signed measure of total mass zero,

we look for those modified rates, i.e., choice of f, such that with the starting measure μ they produce "derivative at time zero" equal to $\dot{\mu}$, i.e.,

$$\dot{\mu}(\sigma) = \sum_i \sum_\alpha (\tilde{r}_\alpha(\tau_i\sigma)\mu(\tau_i T_\alpha \tau_{-i}\sigma) - \tilde{r}_\alpha(\tau_i\sigma)\mu(\tau_i\sigma))$$

The Radon-Nikodym derivative of the path space measure of the finite-volume process (in $\mathbb{T}_d^N$) with rates $\tilde{r}$ w.r.t. the process with rates r is given by the Girsanov formula:

$$\frac{d\mathbb{P}^{[0,T],N}\tilde{r}}{d\mathbb{P}^{[0,T],N}\tilde{r}} = \exp\left(\sum_{i\in\mathbb{T}_d^N}\sum_\alpha\left(\int_0^T \log\frac{\tilde{r}_\alpha^i\sigma_s}{r_\alpha^i(\sigma_s)}dN_s^{i,\alpha} - \int_0^T\left(\tilde{r}_\alpha^i(\sigma_s) - r_\alpha^i(\sigma_s)\right)\right)ds\right)$$

where r_α^i, resp. $\tilde{r}_\alpha^i$ denote the rate to flip from σ to $\tau_i T_\alpha \tau_{-i}(\sigma)$, i.e., to apply the transformation T_α around the lattice site i, and $N_t^{i,\alpha}$ the corresponding counting process counting how many transitions σ to $\tau_i T_\alpha \tau_{-i}(\sigma)$ have happened in the time interval $[0,t]$.

We then find, as in (4.3.10) that the Lagrangian is equal to the limit

$$\Xi(\mu,\dot{\mu}) = \lim_{T\to 0}\frac{1}{T}\lim_{N\to\infty}\frac{1}{|\mathbb{T}_d^N|}s(\mathbb{P}_{\tilde{r},N}^{[0,T]}|\mathbb{P}_{r,N}^{[0,T]})$$

which is the analogue of (4.3.10), replacing relative entropy by relative entropy density.

4.5.6 Diffusion processes: computation of the Lagrangian.

For diffusion processes, let us start with the simplest case of independent diffusions in $d = 1$. The general case will be analogous, but the quadratic forms appearing there will be less explicit. The source generator Q is thus given by

$$Qf(\sigma) = \frac{1}{2}\partial_0^2 f(\sigma)$$

where we abbreviated ∂_0 to denote the partial derivative w.r.t. σ_0. As a consequence, for a local function f:

$$\mathcal{K}_Q f = \sum_k Q(\tau_k f) + \left(\sum_k \partial_0(\tau_k f)\right)^2$$

and, reminding that the full generator is the sum of shifts of Q, we have

$$\mathcal{H}(\mu,f) = \int \mathcal{K}_Q f d\mu = \int \mathcal{L} f d\mu + \mathcal{J}_\mu(f,f)$$

where

$$\mathcal{J}_\mu(f,f) = \int\left(\sum_k \partial_0(\tau_k f)\right)^2 d\mu$$

is a μ dependent quadratic form. This quadratic form is the analogue of (4.4.3). Hence, for the Lagrangian we have

$$\Xi(\mu,\dot\mu)=\sup_f\left(\langle\dot\mu-\mathcal{L}^*\mu,f\rangle-\mathcal{J}_\mu(f,f)\right)=\mathcal{J}^*_\mu(\dot\mu-\mathcal{L}^*\mu,\dot\mu-\mathcal{L}^*\mu)$$

where $\mathcal{J}^*_\mu$ is a dual quadratic form defined via

$$\mathcal{J}^*_\mu(\nu,\nu)=\sup_f(<\nu,f>-\mathcal{J}_\mu(f,f)) \tag{4.5.15}$$

for ν a signed measure of total mass zero. Notice that this indeed defines a quadratic form because for $\lambda>0$ (and with similar derivation for $\lambda<0$)

$$\begin{aligned}\mathcal{J}^*_\mu(\lambda\nu,\lambda\nu) &= \sup_f(\lambda\langle\nu,f\rangle-\mathcal{J}_\mu(f,f))\\ &= \lambda^2\sup_f(\langle\nu,f/\lambda\rangle-\mathcal{J}_\mu(f/\lambda,f/\lambda))\\ &= \lambda^2\mathcal{J}^*_\mu(\nu,\nu)\end{aligned}$$

We see in particular that $\Xi(\mu,\dot\mu)$ is zero for a solution of the Kolmogorov forward equation, i.e., if $\dot\mu=\mathcal{L}^*\mu$, which shows also in the present context that the Markovian evolution of the distribution μ is a zero cost trajectory.

Finally, let us turn to the general case. We split Q, the source generator, into a first order part and a second order part:

$$Q=Q_1+Q_2$$

where Q_2 contains all second order derivatives (variance part of the diffusion), Q_1 all first order derivatives (drift part). To Q_2 is then associated the quadratic form

$$\mathcal{J}^Q_\mu(f,f)=\int\left(e^{-\sum_k\tau_kf}Q_2e^{\sum_k\tau_kf}-Q_2\left(\sum_k\tau_kf\right)\right)d\mu \tag{4.5.16}$$

The Lagrangian is then given by

$$\Xi(\mu,\dot\mu)=(\mathcal{J}^Q_\mu)^*(\langle\dot\mu-\mathcal{L}^*\mu,\langle\dot\mu-\mathcal{L}^*\mu) \tag{4.5.17}$$

where $(\mathcal{J}^Q_\mu)^*$ is the dual quadratic form of $\mathcal{J}^Q$ (as in (4.5.15).

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Summary

In this thesis we use both the two-layer and the large-deviation approach to study the conservation and loss of the Gibbs property for both lattice and mean-field spin systems.

Chapter 1 gives general backgrounds on Gibbs and non-Gibbs measures and outlines the the two-layer and the large-deviation approach. It gives also the overview of the thesis.

Chapter 2 studies the transforms of one-dimensional lattice spin systems. We start from a Gibbs measure with infinite range interaction and consider both deterministic and stochastic transformations K. Using the two-layer approach we prove that the constrained system has a unique Gibbs measure for every choice of transformed configuration, as long as the range of K is finite. This implies that the associated transformed Gibbs measures are always Gibbs. Further, we prove that if the initial interaction is exponentially decaying, then the transformed interaction decays exponentially as well, while if the initial interaction is polynomially decaying (with an exponent large enough so that the system is in the uniqueness regime), then the transformed interaction decays polynomially as well (with a smaller power). The proofs of these results use the house-of-cards coupling argument from Bressaud-Fernández-Galves [1].

Chapters 3 and 4 provide new and explicitly computable examples of Gibbs-non-Gibbs transitions by using the large-deviation approach. These examples include independent Brownian motions, Ornstein-Uhlenbeck processes, and birth-death processes. Chapter 4 computes the Feng-Kurtz Hamiltonian and Lagrangian associated to the large deviations of the trajectory of the empirical distribution for independent Markov processes, and of the empirical measure for translation invariant interacting Markov processes. We treat both the case of jump processes (continuous-time Markov chains and interacting particle systems) and the case of diffusion processes. For diffusion processes, the Lagrangian is a quadratic

[1] X. Bressaud, R. Fernández, A. Galves, Decay of correlations for non Hölderian dynamics, A coupling approach, Electr. J. Prob., 4, 1–19 (1999).

form of the deviation of the trajectory from the Kolmogorov forward equation. In all cases, the Lagrangian can be interpreted as a relative entropy (density) per unit time.

Samenvatting

In dit proefschrift maken we gebruik van zowel de twee-lagen methode als de grote-afwijkingen methode om het behoud en verlies van de Gibbs-eigenschap te bestuderen voor zowel rooster spinsystemen als gemiddelde-veld spinsystemen.

Hoofdstuk 1 presenteert algemene achtergrondinformatie over Gibbs en niet-Gibbs maten en geeft in grote trekken weer wat de beide methoden inhouden.

Hoofdstuk 2 bestudeert de transformaties van een-dimensionale rooster spinsystemen. We starten vanuit een Gibbs maat met een interactie van oneindig dracht en nemen zowel deterministische als stochastische transformaties K in beschouwing. Met behulp van de twee-lagen methode bewijzen we dat het gekoppelde systeem een unieke Gibbs maat heeft voor een willekeurig gekozen getransformeerde configuratie zolang het bereik van K eindig is. Dit impliceert dat de geassocieerde getransformeerde Gibbs maten weer Gibbs zijn. Verder tonen we aan dat de getransformeerde interactie exponentieel (dan wel polynomiaal) vervalt als de initiële interactie exponentieel (dan wel polynomiaal) vervalt, met in het algemeen een kleinere exponent. In het laatste geval moeten de parameters in het uniciteitsregime vallen. De bewijzen hiervan maken gebruik van de kaartenhuis-koppeling van Bressaud-Fernández-Galves [1].

Hoofdstuk 3 en 4 geven nieuwe en expliciet berekenbare voorbeelden van Gibbs-niet-Gibbs overgangen via de grote-afwijkingen methode. Deze voorbeelden zijn onafhankelijke Brownse bewegingen, Ornstein-Uhlenbeck processen, en geboorte-sterfte processen. Hoofdstuk 4 berekent de Feng-Kurtz Hamiltoniaan en Lagrangiaan die geassocieerde zijn met de grote afwijkingen van de baan van de empirische verdeling voor onafhankelijke Markov processen, en van de empirische maat voor translatie-invariante wisselwerkende Markov processen. We behandelen zowel het geval van sprongprocessen (continue-tijd Markov ketens en wisselwerkende deeltjessystemen) als het geval van diffusieprocessen. Voor diffusieprocessen is de Lagrangiaan een kwadratische vorm in de afwijking die

[1] X. Bressaud, R. Fernández, A. Galves, Decay of correlations for non Hölderian dynamics, A coupling approach, Electr. J. Prob., 4, 1–19 (1999).

de baan heeft van de voorwaartse Kolmogorov-vergelijking. In alle gevallen kan de Lagrangiaan geïnterpreteerd worden als een relatieve entropie (dichtheid) per tijdseenheid.

Curriculum Vitae

Feijia Wang obtained his bachelor degree in computer science and technology in 2002 at Shanghai Jiao Tong University and his master degree in applied mathematics (track financial engineering) in 2006 at University of Twente. He has worked as a sales engineer from 2002 to 2003 at BEA Systems, Inc. (now part of Oralce Corporation), as a derivatives researcher from 2006 to 2008 at the Group Risk Management of ABN AMRO Bank, and as a graduate student from 2008 to 2012 at the Mathematisch Instituut of Leiden University.