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Mathematical Physics

Irreversible Parallel Dynamics in Statistical Mechanics

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Summary

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Résumé

In this thesis we present theoretical and numerical approaches for two irreversible and parallel dynamics on one-dimensional statistical mechanics models. In the first chapter we present theoretical results on a particles system driven by an irreversible Markov chain namely the Totally Asymmetric Simple Exclusion Process (TASEP). Allowing multiples spin-flips in each time-step we define a model with a parallel dynamics that belongs to the family of the Probabilistic Cellular Automata (PCA) and we derive its stationary measure. In this framework we deal with *the blockage problem*, *i.e.* to understand the effects of a localized perturbation in the transition rates of the particles on irreversible systems. We find an exact expression of the current with respect to the blockage intensity ε in the deterministic regime of the dynamics.
In the second chapter we present a one-dimensional version of the Ising model with Kac potential. Again we define a PCA dynamics with asymmetric interaction between particles and we find its stationary measure for periodic boundary condition. Then we prove the convergence, in the thermodynamic limit, of such stationary measure to the Gibbs measure for all temperatures above the critical one via Föllmer estimates and Dobrushin's Uniqueness Theorem.
In the second part of the thesis, we investigate these two dynamics through numerical experiments. In the case of the TASEP we exploit general purpose Graphical Processors Unit (GPGPU) writing a parallel code in CUDA to identify a reasonable *mixing time* and reinforce the conjecture that in both version, serial or parallel update rule, the current may be non-analytic in the blockage intensity around the value $\varepsilon = 0$. In the case of the Kac-Ising model we perform statistics to compute the average mixing time for serial dynamics with respect to the temperature β and the interaction length γ^{-1}. Running a self-developed program on 64 processors in parallel we obtained the coalescence times for 20000 samples of trajectories for volume of size 5000. The results show that increasing γ^{-1} and β the irreversible dynamics reaches its equilibrium quicker than the reversible one. A fact that opens new insights of theoretical researches and motivates the study of approaches like parallelism and irreversibility for low temperatures regimes.
The work regarding the PCA-TASEP model has already given a publication: B. Scoppola, C. Lancia, and R. Mariani, *On the blockage problem and the non-analyticity of the current for parallel tasep on a ring*, Journal of Statistical Physics, **161** (2015), pp. 843–858.

Dans cette thèse, nous présentons des approches théoriques et numériques pour deux dynamiques irréversibles et parallèles sur des modèles de mécanique statistique. Dans le premier chapitre, nous présentons les résultats théoriques sur un système de particules induite par une chaîne de Markov irréversible, à savoir le "Totally Asymmetric Simple Exclusion Process" (TASEP). Permettant des multiples retournements de spin à chaque iteration, nous définissons un modèle avec une dynamique parallèle appartenant à la famille des Automates Cellulaires Probabilistes (PCA) et nous dérivons sa mesure stationnaire. Dans ce cadre, nous traitons *le problème du blocage*, *i.e.* comprendre les effets d'une perturbation localisée dans le taux de transition des particules sur des systèmes irréversibles. Nous trouvons une expression exacte du courant par rapport à l'intensité du blocage ε dans le régime déterministe de la dynamique.
Dans le deuxième chapitre, nous présentons une version unidimensionnelle du modèle d'Ising avec potentiel de Kac. Encore une fois, nous définissons une dynamique PCA avec une interaction asymétrique entre particules et nous trouvons sa mesure stationnaire avec condition aux limites périodique. Ensuite, nous prouvons la convergence, dans la limite thermodynamique, de cette mesure stationnaire vers la mesure de Gibbs pour toutes les températures supérieures à la température critique via les estimations de Föllmer et le théorème d'unicité de Dobrushin.
Dans la seconde partie de la thèse, nous étudions ces deux dynamiques à travers des expériences numériques. Dans le cas du TASEP, nous exploitons une unité de processeurs graphiques (GPU) en écrivant un code parallèle dans CUDA pour identifier une estimation raisonnable du temps de mélange et renforcer la conjecture qu'à la fois dans la version, la règle de mise à jour série ou parallèle, le courant peut ne pas être analytique dans l'intensité du blocage autour de la valeur $\varepsilon = 0$. Dans le cas du modèle de Kac-Ising, nous établissons des statistiques pour calculer le temps de mélange moyen de la dynamique en série par rapport à l'inverse de la température β et la longueur de l'interaction γ^{-1}. En exécutant un programme auto-développé sur 64 processeurs en parallèle, nous avons obtenu les temps de coalescence pour 20000 d'échantillons de trajectoires pour un volume de 5000 sites. Les résultats montrent que, dans la dynamique irréversible lors de l'augmentation de γ^{-1} et β l'obtention de l'équilibre est plus rapide que celle de la dynamique réversible. Un fait qui ouvre de nouvelles perspectives de recherches théoriques et motive l'étude d'approches comme le parallélisme et l'irréversibilité pour les régimes de basses températures.
Les travaux concernant le modèle PCA-TASEP ont déjà donné lieu à une publication:
B. Scoppola, C. Lancia, and R. Mariani, *On the blockage problem and the non-analyticity of the current for parallel tasep on a ring*, Journal of Statistical Physics, **161** (2015), pp. 843–858.

Chapter 1

Non-equilibrium steady states for PCA-TASEP

1.1 Introduction

The Totally Asymmetric Simple Exclusion Process (TASEP from here on) is a driven lattice gas with hard-core exclusion and one of the most popular example of Markov irreversible dynamics of a discrete particle system [41, 42]. It is a special case of the Simple Exclusion Process (SEP) introduced by Spitzer in 1970 as a purely mathematical tool for studying the interaction of Markov processes [59]. The SEP model is the natural evolution of random walks on the lattice $\mathbb{Z}^d$ with a hard-core interaction which allows at most one particle per site. In one dimension each particle jumps, independently of the others, to one of its neighbouring sites with fixed probabilities $p, q \geq 0$, $p + q = 1$, unless such target site is already occupied by another particle.
The asymmetric version (ASEP) simply states that the probabilities p, q of the left and right jump are not equal resulting in particles hopping in one direction more often than in the other one. The continous time dynamics assumes that each particle waits a random exponent mean one amount of time and then attempts to jump to its neighbour right site with probability p and to its neighbour left site with probability q, but the jump is performed only if there is no particle at the target site. Otherwise, nothing happens and the particle waits another exponential time.
The model has been used to study a wide variety of physical phenomena such as: transport of macromolecules through thin vessels [40], hopping conductivity in solid electrolytes [53], traffic flow [56] surface growth [27] [35], sequence alignment [9] and molecular motors [33]. Its fortune is due to the fact that the ASEP admits exact analytical solutions (see e.g. [24]) and has important relations to diffusion and growth processes, and to the Kardar–Parisi–Zhang equation [5].
The TASEP represents the limit case of the ASEP where one of the "jump"

parameters, say q, is constantly set to zero. First applied in [49] and [55] to the analysis of vehicular traffic flow it rapidly became a paradigm in Non-Equilibrium Statistical Mechanics [34]. In finite space the system can be defined either on a discrete segment $\Lambda = \{1, 2, ..., 2L\}$ or on a discrete torus (in one dimension a circle) imposing periodic boundary conditions. A configuration $\sigma \in \{0, 1\}^{\Lambda}$ can be viewed as a set of particles living in Λ, *i. e.* a sequence of occupied and unoccupied sites. According to this map, $\sigma_i = 1$ means that the i-th site is occupied by a particle, whereas if $\sigma_i = 0$ then the i-th site is a hole, *i. e.* it is an empty site.
The discrete time dynamics is, again, rather simple: at every time-step a particle is chosen uniformly at random and then it is moved to the site at its right if another particle is not already there. If such site is occupied the configuration remains unchanged and a new particle is chosen.
In spite of having a pretty straightforward definition the model proved to be rich in interesting behaviours giving important results regarding the study of Non-Equilibrium Stationary States (NESS), a compelling theme in statistical mechanics.
It is possible to generalize the dynamics extending the definition to the continuous time on the whole $\mathbb{Z}$ but already in its simplest version this model has several interesting features. On a finite circle the stationary measure is uniform because it's easy to show that its transition matrix is doubly Markov. On the finite segment, instead, the stationary state depends on the boundary rates of the particles to enter (say on the left) and exit (on the right) from the lattice (see [17] [57]).
An interesting quantity to study is the *current* defined as the thermodynamic limit of the average number of free particles, *i. e.* lattice-sites occupied by a particle followed by an empty site. This quantity is important because it measures the tendency of the system to exhibit congestion, *i. e.* its susceptibility to form long sequences of clustered particles that are not free to move. The current is an indication of how fast particles get transported around the ring, thus it is strongly related to the conductivity of the system. A current sensibly smaller than the maximum value means that the typical NESSs exhibit portions of the lattice proportional to its volume that are occupied by clusters of enqueued particles and portions that are not occupied by particles. Very recently, Scoppola et al. have given in [58] a simple and clear derivation of both the stationary distribution and the expression of the current for the PCA-TASEP on a ring. An equivalent definition for the current is that it is the stationary probability that the site i is occupied by a particle and the site $i + 1$ has none. Remarkably, the current does not depend on i and can be exactly computed for both the classical TASEP defined on the segment and on the discrete circle.
In particular, on the discrete circle the current depends only on the number of particles and in the case of half-filled system, *i. e.* when there are L particles in the lattice $\Lambda = \{1, 2, ..., 2L\}$, its maximum is equal to $1/4$ in

the limit $L \to \infty$. On the finite segment the system exhibits a non-trivial behaviour. In fact the stationary current is strongly related to the probability of a particle entering (α) or exiting (β) the system, which has a rich phase diagram in the $\alpha - \beta$ plane, obtained by the "matrix ansatz" (see [17] [57]).
One of the main objective of this thesis is to investigate on a very natural question in the study of the irreversible system: whether the effect of small perturbations in the dynamics has local , as in the case of reversible system far from critical points, or global effects. In the case of the TASEP this question has been investigated imposing the so-called *blockage* or *slow bond* ([29, 28]), *i. e.* in a defined point of the lattice (say in the point $2L$ of the circle w.l.o.g.) the probability of the jump of a particle is reduced to $1 - \varepsilon$, where $0 \leq \varepsilon \leq 1$.
It was long debated whether the presence of such localized perturbation has global effects only for some critical value $\varepsilon_c \geq 0$. Numerical simulations show that the macroscopic value of the current remain unchanged for values of ε close to 0 and, among physicists, a vast range of values $\varepsilon_c > 0$ were proposed. The question came to be known as the "slow bond problem" and for decades it remained unsettled until recently Basu, Sly and Sidoravicius proved in [3] that such critical value is indeed 0 and the effects of the blockage are global for every value of $\varepsilon \geq 0$. Another paper followed, again by Basu et al. [2], focusing directly on the TASEP with a slow bond. Using the connection between TASEP and directed last passage percolation on $\mathbb{Z}^2$ it is proved that the introduction of the blockage has a long range effect on the distribution of the density of particles. There is, therefore, strong indication that the current may decrease, for small ε, with a non analytical dependence on ε (see [13]) but unfortunately the conjecture remains unproven and probably will be object of further research.
A recent development in the study of non-equilibrium properties of irreversible dynamics on a lattice is represented by the employment of Probabilistic Cellular Automata (PCAs). The essential characteristic of these Markov chains is to have an update rule which admits a product form making them, among other things, eligible for large-scale simulative studies on parallel architectures like Graphical Processing Units (GPUs). Dai Pra et al. in [15] applied this class of agent-based dynamics to the Ising model on a lattice with remarkable results. Penalizing the transitions in which too many spins flip simultaneously with an inertial term $q \geq 0$, they showed that if such q is sufficiently strong the PCA dynamics possess a unique stationary distribution that is Gibbsian in the thermodynamic limit.
This result holds true even in certain cases where the PCA is designed to violate the detailed balance principle as shown by Lancia and Scoppola in [37]. That is to say, in a certain region of the parameters the PCA is a model for NESS at all finite sizes, but it behaves like an Equilibrium System in the thermodynamic limit.
In this chapter we present a parallel version of the single-spin dynamics of the

TASEP which fits into such class of PCAs presented in [15]. Indeed, at each time-step each particle followed by an empty site has a finite probability p to jump, therefore the probability of a large number of free particles hopping in the clockwise direction is penalized with an exponentially small inertial weight.
The amount of particles is constrained to be strictly less than the size of the lattice and each site can be occupied by a single particle at most. Particles may hop in the clockwise (counterlockwise w.l.o.g.) direction only and the movement is allowed only if the adjacent site is empty (hard-core exclusion). If, at a certain time, the number of free particles is f, then the number of hopping particles is governed by a binomial law $Bin(f, p)$. Due to its binomial nature it is easy to see that the transition probability from one state to another can be factorized on the single site of the lattice. Hence this parallel dynamics is named PCA-TASEP.
The model was first studied on a ring by Nagel and Schreckenberg [49] as a collective dynamics for freeway traffic and then extended by Schreckenberg et al. [55] to the case of particles performing jumps of length corresponding to their velocity. In the case of jumps limited to next-neighbouring sites (velocity 1), the authors derived through a mean-field approximation the steady-state distribution of the model. However, their derivation is quite involved, requiring to prove that the first order mean-field approximation remains valid at all higher orders. The case of the PCA-TASEP on a ring with inhomogeneous jump-rates is studied in [20], where the stationary distribution of the model is given in a form equivalent to [55]. Schadschneider gives a review of parallel TASEP on a ring with a focus on traffic applications in [54]. An exact solution to PCA-TASEP with open boundary conditions is given both by de Gier and Nienhuis in [16], and by Evans et al. in [20] in terms of a matrix product. An alternative, combinatorial expression in term of Catalan numbers can be found in [19]. Finally parallel TASEP models have been investigated also via Bethe Ansatz imposing both open and periodic boundary. The results obtained so far comprehend the expression of the evolute measure of the model at every time, see for instance [51] [52][44].
In this chapter we will show how, despite the changes, the PCA-TASEP exhibits similar features with respect to the standard TASEP, particularly for what concerns the current and the blockage problem. Numerically, for every $p < 1$ the behaviour of the current is very similar to the serial TASEP because for small ε the macroscopical current appears to be equal to the unblocked one. In the case $p = 1$, on the other side, the system is exactly solvable and it will be proven that $\varepsilon_c = 0$.

1.2 Definitions

We define a Markov chain on a discrete circle, *i. e.* on the set $\Lambda = \{1, 2, ..., 2L\}$ with periodic boundary conditions. As in the case of standard TASEP, a configuration σ is a point in the space phase $S = \{0, 1\}^{\Lambda}$. We will denote with σ_i the local configuration of σ in the point i and we will say that in the site i there is a particle if $\sigma_i = 1$, while we will say that the site i is empty, or equivalently that in the site i there is a hole, if $\sigma_i = 0$. We will say that in i we have a particle free to move if $\sigma_i = 1$ and $\sigma_{i+1} = 0$ and that to move a particle means to substitute the values $\sigma_i = 1$ and $\sigma_{i+1} = 0$ with $\sigma_i = 0$ and $\sigma_{i+1} = 1$.
Each configuration σ can be decomposed into trains of particles, namely sequences of particles lying in consecutive sites. The *engine* of a train is the rightmost element of the sequence with highest index possible with respect to the other particles of the train. The *caboose* is, conversely, leftmost element and has the lowest index. If the train has length bigger than 1 and crosses the boundary of the ring (two of its particles occupy sites 1 and $2L$) its engine and caboose are the elements with smallest and highest index, respectively. Clearly, engines are the only particles with a hole in front of them hence they can move across a single iteration of the dynamics. Whenever an engine is moved it may either form a new train of length 1 or become the caboose of another train.

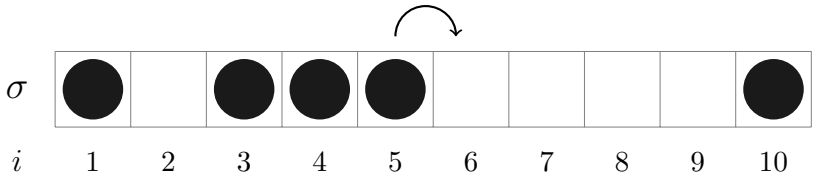

Figure 1.1: Example of transition from configuration σ to τ by the jump of particle in position $i = 4$. The jump makes the *engine particle* in $i = 4$ to detach from its train (from site 2 to 4) and form a new train of length 1. The other train represents the case where the *caboose* has an index greater than the *engine* since it crosses the boundary of the ring, between site 9 and 0.

Given a configuration σ we will define the number of particles in the system as

$$m(\sigma) = \sum_{i=1}^{2L} \sigma_i \tag{1.2.1}$$

and we will assume, from now on, that $m(\sigma) \leq L$. The dynamics conserves the number of particles in Λ, *i. e.* $m(\sigma) = m(\tau) = m$. We will, also, denote with $l(\sigma) \leq m(\sigma)$ the number of particles free to move in the configuration σ, which is clearly equal to the number of particle trains in σ.

We now define the weight of the transition from a configuration σ to a

configuration τ in the following way

$$w(\sigma,\tau) = \begin{cases} w^n & \text{if } \tau \text{ can be reached by } \sigma \text{ moving } n \text{ particles,} \\ 0 & \text{otherwise} \end{cases} \tag{1.2.2}$$

where $w > 0$ is a positive parameter measuring the tendency to move of each particle.
The transition probabilities are therefore

$$P(\sigma,\tau) = \frac{w(\sigma,\tau)}{w(\sigma)} \ , \tag{1.2.3}$$

where

$$w(\sigma) = \sum_{\tau} w(\sigma,\tau) = \sum_{k=1}^{l(\sigma)} \binom{l(\sigma)}{k} w^k = (1+w)^{l(\sigma)} \ . \tag{1.2.4}$$

We call this Markov chain a PCA-TASEP.
With respect to the standard TASEP, where the sequential update rule allows one particle jump per time-step, in the PCA-TASEP at each time-step every particle free to move jumps forward with independent probability $p = {}^{w}/_{1+w}$. In the limit $w \to \infty$, $p = 1$, all free particles move simoultaneously at each time-step, while in the case $w \ll {}^{1}/_{L}$ the model returns to behave like a sequential TASEP.
Being the Markov chain evidently irreducible and aperiodic and having some states τ such that $P_{\sigma,\tau} > 0$ while $P_{\tau,\sigma} = 0$, this Markov chain is visibly irreversible, hence, the *detailed balance principle* cannot be applied to compute explicitly the stationary measure of the dynamics. It is possible, however, to see that for all configurations σ a more general version of the *detailed balance* is satisfied, *i. e.*

$$\sum_{\tau} w(\sigma,\tau) = \sum_{\tau'} w(\tau',\sigma) \tag{1.2.5}$$

known in literature as *global balance principle* or *dynamical reversibility* (see for instance [37]). The proof of (1.2.5) works as follows: for each sequence of consecutive 1s, *i. e.* a train of particles, there is one right endpoint, an *engine* of the train, and respectively, one left endpoint, a *caboose*. Since every train has exactly one *engine* and one *caboose* the final configurations τ at the left hand side of (1.2.5) can be mapped one-to-one onto the initial configurations τ' at the right hand side in such a way that $w(\sigma,\tau) = w(\tau',\sigma)$. More precisely, let τ be the configuration obtained from σ by advancing the *engine* of some particle trains to the empty neighboring sites; similarly, let τ' the configuration obtained from σ by detaching the *caboose* of the very same set of particle trains; clearly, $w(\sigma,\tau) = w(\tau',\sigma)$ since the number of

particles free to move $l(\cdot)$ is equal to the number of trains which is the same for τ and τ'.
The *dynamical reversibility* implies that the stationary measure of the dynamics is

$$\pi(\sigma) = \frac{w(\sigma)}{\sum_\sigma w(\sigma)} \tag{1.2.6}$$

since it's easy to see that it satisfies the definition of stationary measure, *i. e.*

$$\begin{aligned}\sum_\sigma \pi(\sigma)P(\sigma,\tau) = \sum_\sigma \frac{w(\sigma)}{W}\frac{w(\sigma,\tau)}{w(\sigma)} &= \sum_\sigma \frac{w(\sigma,\tau)}{W} \\ &= \sum_\sigma \frac{w(\tau,\sigma)}{W} = \frac{w(\tau)}{W} = \pi(\tau)\ .\end{aligned} \tag{1.2.7}$$

Defining the normalization factor for $\pi(\sigma)$ as follows

$$W := \sum_\sigma w(\sigma) \tag{1.2.8}$$

and using the relation in (1.2.4) such stationary measure can be expressed as

$$\pi(\sigma) = \frac{(1+w)^{l(\sigma)}}{W}\ . \tag{1.2.9}$$

Looking at the expression of (1.2.9) one notes that when the weight of the transition $w \to 0$, when particles jumps very rarely, the stationary measure tends to the uniform measure

$$\pi(\sigma) = \frac{1}{\binom{2L}{m(\sigma)}}\ . \tag{1.2.10}$$

That completely agrees with the serial TASEP case. In fact, imposing $w \to 0$ implies that the jump of more than one particle at once is very unlikely, and we return to the single spin-flip dynamics of the standard TASEP which has a uniform stationary distribution.
In the limit $w \to \infty$, *i. e.* $p = 1$, the situation is radically different. Since we supposed that $m(\sigma) \leq L$, the maximum number particles free to move is $m(\sigma)$, hence, in this regime, the leading order of W is $w^{m(\sigma)}$ and all configurations with $l(\sigma) < m(\sigma)$ have a weight smaller by at least a factor $1/1+w$. Being the probability of the jump $p = 1$ every initial congestion in the lattice vanishes after at most $m(\sigma)$ time-steps and we arrive to a configuration with $l(\sigma) = m(\sigma)$. After that, all particles continue to move forward and no new traffic jam forms. Thus, the stationary measure tends to be uniform on all the configurations where the number of particles free to move $l(\sigma)$ is equal to total number of particles $m(\sigma)$.

1.3 Current for the half-filled PCA-TASEP

As discussed in the introduction, indicating with π^{S} the stationary measure of the dynamics, the current J^{S} for the sequential TASEP model is defined as

$$J^{\mathrm{S}} := \lim_{\Lambda\to\infty} \pi^{\mathrm{S}}(\sigma_i = 1, \sigma_{i+1} = 0). \tag{1.3.1}$$

Equivalently, it can be defined as follows

$$J^{\mathrm{S}} := \lim_{\Lambda\to\infty} \frac{\mathbb{E}_{\pi^{\mathrm{S}}}[l(\sigma)]}{2L} \tag{1.3.2}$$

i. e. the thermodynamic limit of the expectation of the number of free particles $l(\cdot)$ with respect to π^{S}.
Probability (1.3.1) is independent of the site i while it depends on the total number of particles $m(\sigma)$. From now on, we consider the half-filled case in which $m(\sigma) = L$, *i. e.* the number of particles is exactly half of the number of sites. In such a case, for the standard TASEP, the current is

$$J^{\mathrm{S}} = \pi^{\mathrm{S}}(\sigma_i = 1, \sigma_{i+1} = 0) \sim \pi^{\mathrm{S}}(\sigma_i = 1) \cdot \pi^{\mathrm{S}}(\sigma_{i+1} = 0) = \frac{1}{4}$$

since the stationary probability π^{S} is uniform and therefore the probability to have the configuration $\sigma_i = 1, \sigma_{i+1} = 0$ tends for large Λ to be simply the product of the two independent probabilities to have $\sigma_i = 1$ and $\sigma_{i+1} = 0$, both equal to $1/2$.
For the PCA-TASEP we can analogously define the current J^{P} as

$$J^{\mathrm{P}} := \lim_{\Lambda\to\infty} \pi^{\mathrm{P}}(\sigma_i = 1, \sigma_{i+1} = 0) = \lim_{\Lambda\to\infty} \frac{\mathbb{E}_{\pi^{\mathrm{P}}}[l(\sigma)]}{2L} \ . \tag{1.3.3}$$

Then the following result holds:

Proposition 1.3.1. The value of the current $J^{\mathrm{P}} = \lim_{\Lambda\to\infty} \pi(\sigma_i = 1, \sigma_{i+1} = 0)$ for the irreversible Markov chain defined by the transition probabilities in (1.2.3) is given by

$$J^{\mathrm{P}} = \frac{1}{2} \ \frac{\sqrt{1+w}}{1+\sqrt{1+w}} \ . \tag{1.3.4}$$

Proof. We rewrite J^{P} in the following form

$$J^{\mathrm{P}} = \lim_{L\to\infty} \frac{1}{2L} \ \frac{\sum_\sigma l(\sigma)(1+w)^{l(\sigma)}}{\sum_\sigma (1+w)^{l(\sigma)}} = \lim_{L\to\infty} \frac{1}{2L} \ \frac{\sum_{l=1}^{L} l \ n(l)(1+w)^l}{\sum_{l=1}^{L} n(l)(1+w)^l} \tag{1.3.5}$$

where $n(l)$ is the number of configurations σ having $l(\sigma) = l$ particles free to move. We have therefore to count such $n(l)$.
First we note that fixed the state of one site, say $\sigma_1 = 1$, a configuration is uniquely determined by the alternate sequence of particle-trains and hole-trains. Then we have to count the number of ways for dividing L particles in

l distinct particle-trains and L holes in l hole-trains which is $\binom{L-1}{l-1}$ since L objects can be divided in l groups. If, then, we suppose that the first train of particles has length l_1, then there are l_1 ways for the site $i=1$ to belong to the first particle-train and $l_1\binom{L-l_1-1}{l-2}$ ways we can have l trains of which the first has l_1 particles. We then multiply by 2 to take into account the configurations having $\sigma_1=0$ and we get

$$n(l) = 2\sum_{l_1=1}^{L-l+1} l_1 \binom{L-l_1-1}{l-2}\binom{L-1}{l-1} . \tag{1.3.6}$$

If we put (1.3.6) into (1.3.5) we get

$$J^{\mathrm{P}} = \lim_{L\to\infty}\frac{1}{2L}\,\frac{\sum_{l=1}^{L}\sum_{l_1=1}^{L-l+1} l_1\binom{L-l_1-1}{l-2}\binom{L-1}{l-1}\; l\;(1+w)^l}{\sum_{l=1}^{L}\sum_{l_1=1}^{L-l+1} l_1\binom{L-l_1-1}{l-2}\binom{L-1}{l-1}(1+w)^l} . \tag{1.3.7}$$

In order to evaluate (1.3.7) we write $l=\alpha L$, $l_1=\alpha_1 L$ and we use the leading order approximation

$$\binom{n}{\alpha n} \approx e^{nI(\alpha)} \tag{1.3.8}$$

where $I(\alpha) = -\alpha\ln\alpha - (1-\alpha)\ln(1-\alpha)$.
Then we get

$$J^{\mathrm{P}} = \lim_{L\to\infty}\frac{1}{2L}\; L\frac{\int_0^1 d\alpha\int_0^{1-\alpha} d\alpha_1\;\alpha\;\alpha_1 e^{L\left((1-\alpha_1)I(\frac{\alpha}{1-\alpha_1})+I(\alpha)+\alpha\ln(1+w)\right)}}{\int_0^1 d\alpha\int_0^{1-\alpha} d\alpha_1\;\alpha_1 e^{L\left((1-\alpha_1)I(\frac{\alpha}{1-\alpha_1})+I(\alpha)+\alpha\ln(1+w)\right)}} . \tag{1.3.9}$$

Calling now

$$f(\alpha,\alpha_1) = (1-\alpha_1)I\left(\frac{\alpha}{1-\alpha_1}\right) + I(\alpha) + \alpha\ln(1+w) \tag{1.3.10}$$

we proceed using the saddle point method to write

$$J^{\mathrm{P}} = \lim_{L\to\infty}\left[\frac{1}{2}\bar{\alpha} + O\left(\frac{1}{L}\right)\right] \tag{1.3.11}$$

where $\bar{\alpha}$ is the value of α that maximizes $f(\alpha,\alpha_1)$. The latter is easy to identify because computing

$$\frac{\partial}{\partial\alpha_1} f(\alpha,\alpha_1) = \log\frac{\alpha+\alpha_1-1}{\alpha_1-1} \tag{1.3.12}$$

we see that $f(\alpha,\alpha_1)$ is decreasing in α_1 and impose $\alpha_1\geq 0$. Thus, choosing $\alpha_1=0$, we get

$$f(\alpha) = 2I(\alpha) + \alpha\ln(1+w) \tag{1.3.13}$$

and computing

$$\frac{d}{d\alpha} f(\alpha) = -2\ln(\alpha) + 2\ln(1-\alpha) + \ln(1+w) \tag{1.3.14}$$

it's easy to see that $f(\alpha)$ is maximized by

$$\bar{\alpha} = \frac{\sqrt{1+w}}{1+\sqrt{1+w}} \ . \tag{1.3.15}$$

Substituting $\bar{\alpha}$ in (1.3.11) we obtain the following expression for the current in the PCA-TASEP

$$J^{\mathrm{P}}(w) = \frac{1}{2} \ \frac{\sqrt{1+w}}{1+\sqrt{1+w}} \ . \tag{1.3.16}$$

□

Note that for $w = O\left(1/L\right)$ we have that, as expected, $J^{\mathrm{P}} = \frac{1}{4}$ as in the sequential TASEP. Such current is an increasing function of w giving $J^{\mathrm{P}} = \frac{1}{2}$ for $w \to \infty$.

1.4 An (easy) blockage problem for the half-filled PCA-TASEP

As discussed in the introduction, a very interesting and difficult open problem in non-equilibrium statistical mechanics is to establish if a localized perturbation of arbitrarily small intensity in the dynamics has macroscopical effects on the system. In the case of the TASEP such question has been investigated by means of the so called "blockage problem", see for reference [42], [29], [13], [2].
The PCA-TASEP version of the *blockage problem* works as follows. The dynamics is defined by the fact that at each time-step a particle in the site $i \in \Lambda$ is chosen uniformly at random and if it is free to move it jumps to its right neighboring site with probability p for every site $i \neq 2L$. If there is a particle in $i = 2L$ and it is free to move (*i. e.* if $\sigma_{2L} = 1$ and $\sigma_1 = 0$), it is moved with probability $p(1-\varepsilon)$, where $\varepsilon \in [0,1]$.

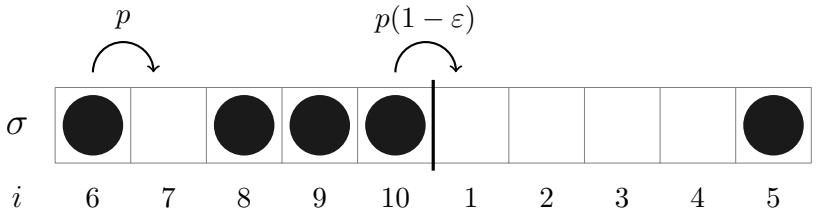

Figure 1.2: PCA-TASEP with blockage dynamics. Every particle free to move jumps forward with probability p except the particle in $i = 2L$ which jumps with probability $p(1-\varepsilon)$ where $\varepsilon \in [0,1]$.

An explicit expression for the current is not yet known neither for the serial nor for the parallel TASEP with blockage. Numerical and perturbative arguments show that, considering always the half-filled case in which the number of particles is $m(\sigma) = L$, the current seems to remain equal to its maximum value $J = \frac{1}{4}$ until a critical value of ε. However, the results in [3] and [2] prove that $J(\varepsilon)$ is strictly less than its maximum value $1/4$ for every value of the blockage intensity $\varepsilon > 0$, settling $\varepsilon_c = 0$. It remains an open question whether the expression of J as a function of ε behaves as a very high-order polynomial around the value $\varepsilon = 0$, or if it has an essential singularity in $\varepsilon = 0$, as conjectured in [13].
To treat analytically the blockage problem in the context of the PCA-TASEP we do the following. Define the weight of the transition from the configuration σ to the configuration τ by

$$w_\varepsilon(\sigma,\tau) = \begin{cases} w^n\big(1-\varepsilon \mathbb{1}_{\{\sigma_{2L}=1,\tau_{2L}=0\}}\big) & \text{if } \tau \text{ can be reached by } \sigma \\ & \text{moving } n \text{ particles,} \\ 0 & \text{otherwise,} \end{cases} \tag{1.4.1}$$

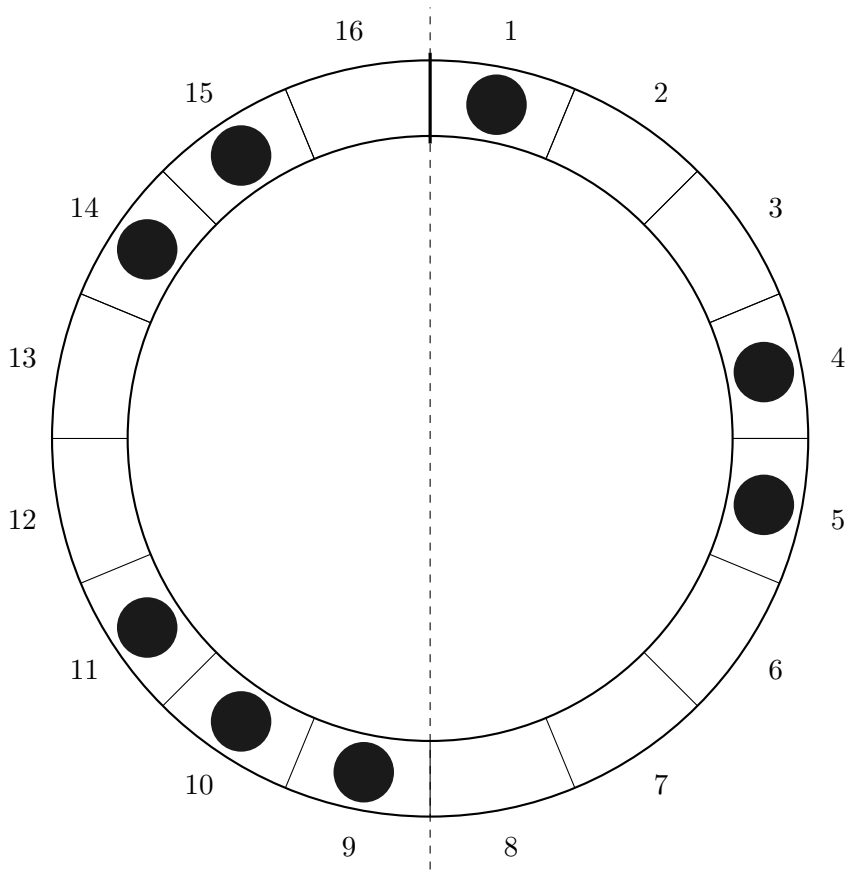

Figure 1.3: Example of particle-hole symmetric configuration: $\sigma_i = 1 - \sigma_{-i} \forall i$. The vertical axis symmetry is due to the presence of the blockage between site $2L = 16$ and site 1.

where $\mathbb{1}_{\{\sigma_{2L}=1,\tau_{2L}=0\}}$ is equal to 1 if both conditions $\sigma_{2L}=1$, $\tau_{2L}=0$ are verified, and is 0 otherwise.
Thus, the transition probabilities for the PCA-TASEP with blockage are

$$P_\varepsilon(\sigma,\tau)=\frac{w_\varepsilon(\sigma,\tau)}{w_\varepsilon(\sigma)} \tag{1.4.2}$$

where

$$w_\varepsilon(\sigma)=\sum_\tau w_\varepsilon(\sigma,\tau)\ . \tag{1.4.3}$$

In this case the presence of the blockage in the point $2L$ results in the fact that the global balance principle is not longer satisfied by the chain. Therefore, finding the stationary measure becomes extremely difficult.
From a numerical point of view the dynamics appears to be similar to the classical TASEP case: the current seems to be constant until ε reaches a critical value, which is a decreasing function of w. The possibility of rigorously proving any result about this behaviour seems nevertheless to be as hard as for the serial dynamics.
There is, however, an exception, which is the regime $w\to\infty$, *i. e.* the case in which *all* the particles free to move actually jump forward with probability $p=1$, except the particle in the site $2L$ which moves with probability $1-\varepsilon$. This case is easy to solve due to the property of the dynamics to preveserve the so-called *particle-hole symmetry*, showed in Figure 1.3 and defined next.
Remark: In the following we allow for negative indexing of the configuration σ under the convention that $\sigma_{-i}=\sigma_{2L-i+1}$.

Definition 1.4.1. A configuration σ such that, for all $i=1,2,...,L$, $\sigma_i=1-\sigma_{-i}$ is said to be *particle-hole symmetric*. Let us denote with PH the set of all the particle-hole symmetric configurations.

In the limit $w\to\infty$ the dynamics preserves such particle-hole symmetry.

Lemma 1.4.1. Consider the transition probabilities

$$P_{\varepsilon,\infty}(\sigma,\tau)=\lim_{w\to\infty}P_\varepsilon(\sigma,\tau)\ . \tag{1.4.4}$$

For each $0\le\varepsilon<1$ and for each $\sigma\in PH$, if τ is such that $P_{\varepsilon,\infty}(\sigma,\tau)>0$ then $\tau\in PH$.

Proof. Let us fix a site $i\in\{2,3,\dots,L\}$ and start considering the case $\sigma_i=1$. Due to the PH-symmetry, if σ_i is an engine then also σ_{-i-1} is an engine; since in the regime $w\to\infty$ the engines move with probability 1, the sites i and $-i-1$ will become holes, *i. e.* $\tau_i=\tau_{-i-1}=0$, while the sites $i+1$ and $-i$ will be occupied by a particle, *i. e.* $\tau_{i+1}=\tau_{-i}=1$. Conversely, if σ_i is not an engine then it must have a particle ahead: $\sigma_{i+1}=1$. Thus, $\sigma_{-i}=\sigma_{-i-1}=0$; therefore, site i will keep being occupied, while site $-i$ will continue being empty, that is to say, $\tau_i=1$ and $\tau_{-i}=0$. The case $\sigma_i=0$ is

completely analogous, *i. e.* we have to distinguish between site i being or not being the caboose of a train of holes which behaves exactly like a train of particles, just in the opposite direction.
We still have to focus to what happens across the blockage on the sites $2L$ and 1 where, among the six possible configurations shown in Figure 1.4, only four are particle-hole symmetric (a. b. c. and d.).
In the case a. site 1 remains occupied and site $2L$ empty, then $\tau_1 = 1$ and $\tau_{-1} = 0$; in the case c. site 1 becomes empty and site $2L$ occupied, then $\tau_1 = 0$ and $\tau_{-1} = 1$. Conversely, in cases b. and d. site 1 becomes occupied and site $2L$ empty with probability $1 - \varepsilon$, *i. e.* $\tau_1 = 1$ and $\tau_{-1} = 0$, or with probability ε the blockage acts on the particle at site $2L$, which remains occupied, *i. e.* $\tau_1 = 0$ and $\tau_{-1} = 1$.
In all these scenarios we have that, after the transition from σ to τ, the configuration τ is such that $\tau_1 = 1 - \tau_{2L}$, hence it fulfills the definition of particle-hole symmetry given in (1.4.1).

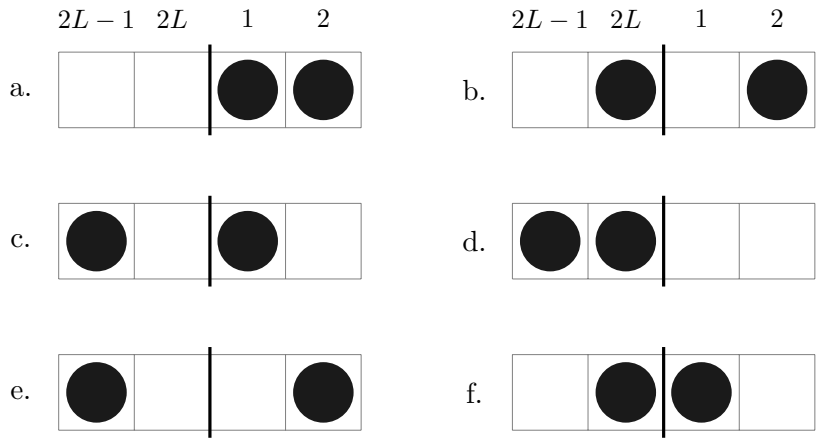

Figure 1.4: Possible configurations partial configurations of the lattice across the blockage, *i. e.* sites $i \in \{2L - 1, 2L, 1, 2\}$. Cases e. and f., represented for completeness, are not particle-hole symmetric hence they play no role in the proof of the lemma.

□

We want, now, to show two lemmata in order to identify the set of recurrent states of our Markov chain $P_{\varepsilon,\infty}(\sigma, \tau)$, but first we need the following definition as presented in [22].

Definition 1.4.2 (Transient State). Calling $P^t_{\sigma\tau}$ the probability to evolve from configuration σ to τ in t time steps, the state $\bar{\sigma}$ is called *unessential* or *transient* if there exist a state $\bar{\tau}$ such that $P^n_{\bar{\sigma}\bar{\tau}} > 0$, but $P^m_{\bar{\tau}\bar{\sigma}} = 0$ for all m.

The defining characteristic of a transient state is the fact that it exists a positive probability to move from it to another one in a finite time, but it is

no longer possible to return there hereafter.

Lemma 1.4.2. For the Markov chain $P_{\varepsilon,\infty}(\sigma,\tau)$ all the states $\sigma \notin PH$ are transient.

Proof. An easy way to prove this lemma is the following observation: for all initial configurations, with a finite probability $p > \varepsilon^{2L}$ the system goes in a time $2L$ in the configuration σ_{queue} such that $\sigma_i = 0$ for $i = 1, 2, ..., L$ and $\sigma_i = 1$ for $i = L+1, L+2, ..., 2L$, *i. e.* if the particle in $2L$ does not move for $2L$ time-steps then all the other particles will be in queue behind it. The state σ_{queue} is of course particle-hole symmetric. Hence starting from any initial state $\sigma \notin PH$ we have a finite probability to arrive in a symmetric state, for instance $\sigma_{\text{queue}} \in PH$ after $2L$ steps, and hence with finite probability we will never visit again σ. □

The next easy but important observation is the following: if the system reached at some time a symmetric configuration $\sigma^\star \in PH$ in which all the particles in the first half of the ring $\{1, 2, ..., L\}$ are free to move, then in that half of the circle all the particles will be free to move at any subsequent time. This is due to the fact that all the particles in $\{1, 2, ..., L-1\}$ can never reach the particle ahead since they all move at any step with probability one. Since $\sigma^\star \in PH$ the particle in $i = L$ is always free to move because $\sigma^\star_L = 1$ implies $\sigma^\star_{-L} = \sigma^\star_{L+1} = 0$ by definition of particle hole symmetry.
We will call Ω_∞ the set of all configurations $\sigma \in PH$ such that all the particles in $\{1, 2, ..., L\}$, even if there is none, are free to move.

Lemma 1.4.3. For the Markov chain $P_{\varepsilon,\infty}(\sigma,\tau)$ all the states $\sigma \notin \Omega_\infty$ are transient.

Proof. Starting from any state $\sigma \notin \Omega_\infty$ the system has a finite probability to reach the configuration σ_{queue} in $2L$ time-steps, and $\sigma_{\text{queue}} \in \Omega_\infty$. The lemma is proved repeating the argument leading to Lemma 1.4.2. □

The stationary probability $\pi_{\varepsilon,\infty}$ of the Markov chain $P_{\varepsilon,\infty}(\sigma,\tau)$ is therefore supported on Ω_∞, where the Markov chain is manifestly ergodic by the reasoning in the proof of Lemma 1.4.2. Call as before

$$J_{\varepsilon,\infty} = \lim_{\Lambda\to\infty} \pi_{\varepsilon,\infty}(\sigma_i = 1, \sigma_{i+1} = 0) \tag{1.4.5}$$

the current with blockage intensity ε and transition weight $w \to \infty$. Let $r(\sigma)$ be the number of particles that lie in first half of the circle, the sites $\{1, 2, ..., L\}$, which, by Lemma 1.4.3, are all free to move. Observing that the number of particles free to move in the second half of the circle $\{L+1, L+$

$2, \dots, 2L\}$ is again $r(\sigma)$ by the particle-hole symmetry, we can compute $J_{\varepsilon,\infty}$, as done in (1.3.3), writing

$$J_{\varepsilon,\infty} = \lim_{L\to\infty} \frac{R}{L} \tag{1.4.6}$$

where $R = \mathbb{E}_{\pi_{\varepsilon,\infty}}(r)$ is the expected value of $r(\sigma)$ with respect to the stationary measure $\pi_{\varepsilon,\infty}$.
We are now ready to prove the fundamental result of this section.

Theorem 1.4.1. The current $J_{\varepsilon,\infty}$ of the Markov chain $P_{\varepsilon,\infty}(\sigma,\tau)$ is given by

$$J_{\varepsilon,\infty} = \frac{1-\varepsilon}{2-\varepsilon}\ . \tag{1.4.7}$$

Proof. The first part of the proof is the computation of the stationary measure of the process. Let us say that at each step in which $\sigma_{2l} = 1$ the blockage is driven by a binary random variable, that can either be *green*, giving in the successive time-step $\tau_{2L} = 0$, or *red*, giving in the successive time-step $\tau_{2L} = 1$. Due to the symmetry we can say that the probability of each configuration can be written in terms of a sequence of green and red lights. In particular, when the particle has passed the blockage, and therefore $\sigma_{2L} = 0, \sigma_1 = 1$, we know that in the next step we will have for sure $\tau_1 = 0, \tau_2 = 1$. Since, by symmetry, $\tau_{2L} = 1 - \tau_{-2L} = 1 - \tau_1 = 1$ this means that we have now a particle in the site $2L$. Hence the presence of a new particle in the set $\{1, 2, \dots, L\}$ is due only to the values of the red light. Let us first consider the set of states $\sigma \in \Omega_\infty$ such that $\sigma_1 = 0$. Then, if site $i \in \{2, \dots, L\}$ is occupied then site $i-1$ is a hole with probability 1. Therefore it is easy to realize that the (stationary) probability to have r particles in $\{1, 2, \dots, L\}$ is

$$\pi_{\varepsilon,\infty}(r) = (1-\varepsilon)^r \varepsilon^{L-2r}. \tag{1.4.8}$$

The exponent $L-2r$ is due to the fact that each green light, with probability $(1-\varepsilon)$, results in one free particle and also an empty site ahead of it.
Conversely, if $\sigma_1 = 1$ then the exponents appearing in (1.4.8) may increase or decrease by a unit at most but this correction is negligible in the thermodynamic limit, thus we will use (1.4.8) to compute the current according to (1.4.6).
For large L we have, therefore

$$R = \mathbb{E}_{\pi_{\varepsilon,\infty}}(r) \approx \frac{\sum_{r=1}^{L/2} r\binom{L-r}{r}(1-\varepsilon)^r\varepsilon^{L-2r}}{\sum_{r=1}^{L/2} \binom{L-r}{r}(1-\varepsilon)^r\varepsilon^{L-2r}}\ . \tag{1.4.9}$$

We can, again, evaluate this sum simply by using the approximation in (1.3.8) and the saddle point method. We call $x = \frac{r}{L}$ and we recast (1.4.9) as

$$R \approx L\frac{\int_0^{L/2} x e^{[L((1-2x)\ln\varepsilon + x\ln(1-\varepsilon) - x\ln\frac{x}{1-x} - (1-2x)\ln\frac{1-2x}{1-x})]}}{\int_0^{L/2} e^{[L((1-2x)\ln\varepsilon + x\ln(1-\varepsilon) - x\ln\frac{x}{1-x} - (1-2x)\ln\frac{1-2x}{1-x})]}} \tag{1.4.10}$$

In the limit $L \to \infty$ we have that

$$J_{\varepsilon,\infty} = \lim_{L\to\infty} \frac{R}{L} \approx \bar{x} \tag{1.4.11}$$

where $\bar{x}$ is the value of x that maximizes

$$f(x) = (1-2x)\ln\varepsilon + x\ln(1-\varepsilon) - x\ln\frac{x}{1-x} - (1-2x)\ln\frac{1-2x}{1-x}\ . \tag{1.4.12}$$

Being

$$\frac{d}{dx}f(x) = -2\ln(\varepsilon) + \ln(1-\varepsilon) - \ln\left(\frac{x}{1-x}\right) + 2\ln\left(\frac{1-2x}{1-x}\right) \tag{1.4.13}$$

we find

$$J_{\varepsilon,\infty} = \bar{x} = \frac{1-\varepsilon}{2-\varepsilon} \tag{1.4.14}$$

which completes the proof. □

Remark 1.4.1. Despite its simplicity, this computation proves, in this completely parallel context, that a very small perturbation of the transition probabilities in a single site extends its effect over all the volume L, without any fading. Indeed, the uniform density of the particles in the set $\{1, 2, \ldots, L\}$ is $\frac{1-\varepsilon}{2-\varepsilon}$ while in the set $\{L+1, L+2, \ldots, 2L\}$ the uniform density is $\frac{1}{2-\varepsilon}$.

Chapter 2

Irreversible parallel Kac-Ising model

2.1 Introduction

The Ising model, proposed by Lenz and solved by Ernst Ising in one dimension in 1925, is one of the simplest theoretical description of ferromagnetism in statistical mechanics. Magnetic dipole moments, *spins* from here on, are defined as discrete variables $\sigma_i \in \{-1, 1\}$ arranged on the sites of a d-dimensional lattice Λ, and interacting among nearest neighbors. The Hamiltonian of such a discrete spin system can be written in the form

$$H(\sigma) = -\sum_{ij} J(i,j)\,\sigma_i\sigma_j \tag{2.1.1}$$

where $i, j \in \Lambda \subset \mathbb{Z}^d$ are the sites of the lattice and $J(i,j)$ is a potential equal to 1 if i, j are nearest neighbors and 0 otherwise.
After Ising's solution, in 1944 Onsager proved in [50] that, differently from the one dimensional case, in the 2-dimensional square lattice the model undergoes phase transitions. From that moment, the model was extensively studied and showed wonderfully rich behaviors in higher dimensions making it the prototypical model for magnetic interactions.
As we said, the classical definition of the Hamiltonian of the Ising model was restricted to consider only the interaction between *nearest neighbors* pairs of sites but this *range* 1 restriction was a major limitation. In fact physics and chemistry models need to cope with long range (possibly infinite) interactions, which however yields to problems in general very hard to solve. The first solution to the issue was the Mean-Field Model that, by reducing the large number of individual interactions to a single averaged effect, allowed to obtain a partly satisfying solution. Indeed, the main issue was the non convexity of the *canonical free energy*.

To improve the situation, in 1963 Kac et al. introduced a new definition of potential $J_\gamma(r) = \gamma J(\gamma r)$ where r is the distance between spins and γ represents the inverse of the range of interaction, see [30]. Such model, in a sense intermediate between short range and mean-field, allowed to prove, among other things, the existence of a critical temperature and explain the phenomenon of spontaneous magnetization in ferromagnetic systems.
Indeed, in 1966 Lebowitz and Penrose derived in a mathematically rigorous way the microscopic van der Waals theory of the liquid-gas transition in [38] and a straightforward generalization of this argument can be found, in the case of discrete spin systems, in [60]. The model was later studied in 1993 by Cassandro, Orlandi and Presutti in [12] in one dimension using a *block-spin* construction which let them analyze the typical profiles at low temperature and give upper and lower bounds of the space scale where these profiles are constant. An analogous investigation but in a disordered version, the so-called Kac-Hopfield model, was realized by Bovier, Gayrard, and Picco in 1995 in [6] and [7].
However, extending the analysis in higher dimensional spaces is non trivial even for the classical Kac-Ising model, see for instance [10] and [8], and even in one dimension the number of open questions that can be addressed is remarkable. Very recently in [11] Cassandro, Merola and Presutti continued the study of the Kac model in one dimension finding, for γ small enough, that the in the infinite volume the coarse grained length of the plus-minus intervals is a renewal process.
It has to be said that the majority of the cited works rely on a purely statical analysis. A different approach is represented by the implementation of a dynamics on the system in order to find the relation between its stationary distribution (equilibrium) and the Gibbs measure. In this setting it becomes interesting to study dynamical features such as the *mixing time*, *i. e.* the time scale needed to get to the equilibrium, and develop numerical simulations to follow the evolution of the system. The Glauber dynamics is the most obvious example of this so-called *Gibbs Samplers* and it's considered to be the most efficient one among the single spin-flip dynamics. An extensive review on the subject can be found in Martinelli's book [45].
In this chapter we deal with this dynamical analysis proposing two Markov chains based on the Hamiltonian (2.1.1) with Kac's potential and we investigate the consequences of *irreversibility* and *parallelism*. That is to say, we define a dynamics where each spin is updated according to the average magnetization of the $\gamma^{-1} \in \mathbb{N}$ spins on its right. Such asymmetrical interaction breaks the time-reversibility of the evolution of the system implying its irreversibility. We also define the transition probabilities in such a way that it is allowed to update multiple spins in the same time-step. This construction belongs to the family of Probabilistic Cellular Automata (PCA), *i. e.* discrete-time Markov chain whose transitional probability is a product measure, see for reference [23].

The interest in such irreversible and parallel approach rises after some remarkable examples of fast convergence times to equilibrium of this kind of dynamics, *e. g.* in [14] is defined an asymptotically polynomial-time approximation scheme for the 2d Ising model. In this case, the high mobility of the parallel updating rule and the asymmetry of the interaction allow to shorten the *tunneling time*, needed for the mixing of the phases. Indeed it is possible to show that such tunneling time becomes polynomial whereas it is exponentially long in the volume in reversible Glauber dynamics, due to *metastability* effects. Hence, this approach seems very promising for the development of a faster and more efficient *sampler* for the Gibbs measure.
In this regards the nature of the parallel update rule, involving only simple operations on many data elements, is particularly suited for implementing numerical simulations on Graphical Processors Unit (GPU) and multi-processors architecture in general. In recent times, the great effort in the improvement of video cards (GPU), their availability at affordable prices, and the advent of parallel computing platforms (API) such as CUDA[1] allowed the scientific computing community to develop the so called General Purpose GPU (GPGPU) paradigm for high-performance computing[2], see for instance [32]. The result is an affordable, highly scalable and efficient way to perform heavy numerical simulations in feasible times, and it is also tested to be more sustainable, in terms of energetic consumption, than the standard CPU computation, see [47]. The aim of this chapter is, therefore, to present dynamics which combine the intrinsic speedup of the irreversible PCAs with the parallel capabilities of the GPGPU.
In Section 2.4 we introduce and study a non-parallel *single spin-flip* update rule with long range interactions between spins. We find its stationary distribution and prove that, if the system is translation invariant, it is the Gibbs measure in both *reversible* and *irreversible* cases using balance equation. In section 3.3, we show how numerical simulations strongly suggest that the irreversible update *mixes* faster than the reversible one. In Section 2.5 we define an actual parallel process (a Probabilistic Cellular Automaton) and we study it in the nearest neighbors case, *i. e.* for $\gamma = 1$, proving it has again the Gibbs measure as stationary distribution at all temperatures. In the general $\gamma < 1$ case we are able to prove that the stationary distribution of such irreversible PCA *tends* to the Gibbs measure in the thermodynamic limit for a suitable choice of parameters (high temperature) via the Föllmer covariance estimate.

[1] https://developer.nvidia.com/cuda-zone
[2] https://hgpu.org/

2.2 Definitions

We consider a one-dimensional lattice Λ of size L with periodic boundary conditions, *i. e.* a ring, where the state of every site $i \in \Lambda$ is represented by a variable $\sigma_i = \{1, -1\}$. Defining the phase space $S = \{-1, 1\}^\Lambda$, a point $\sigma \in S$ will be called the configuration of *magnetic spins* on the ring Λ.
We define the Hamiltonian for such system as follows

$$H_\gamma(\sigma) = -\sum_{i,j\in\Lambda} J_\gamma(i,j)\sigma_i\sigma_j \tag{2.2.1}$$

where $J_\gamma(i,j)$ is the Kac potential between i and j.
Kac potentials are defined as functions $J_\gamma(\cdot)$ such that

$$\sum_{i\in\mathbb{Z}^d} J_\gamma(i,\cdot) = \sum_{j\in\mathbb{Z}^d} J_\gamma(\cdot,j) = 1 \tag{2.2.2}$$

where the parameter $\gamma > 0 : 1/\gamma \in \mathbb{N}$ represents the inverse of the range of interaction. For our purposes we define two kinds of potential.
We will call *symmetric* a potential such that

$$\bar{J}_\gamma(i,j) = \tfrac{\gamma}{2}\mathbb{1}_{\{0<|j-i|\leq 1/\gamma\}} \ . \tag{2.2.3}$$

Conversely an *asymmetric* potential will have the form

$$J_\gamma(i,j) = \gamma\mathbb{1}_{\{0<j-i\leq 1/\gamma\}} \ . \tag{2.2.4}$$

Note that, because the Hamiltonian is the sum over all $i \in \Lambda$, we have

$$H_\gamma(\sigma) = -\sum_{i,j\in\Lambda} \bar{J}_\gamma(i,j)\sigma_i\sigma_j = -\sum_{i,j\in\Lambda} J_\gamma(i,j)\sigma_i\sigma_j \ . \tag{2.2.5}$$

The Gibbs measure on the state space S, with potential $J_\gamma(i,j)$ and inverse temperature $\beta > 0$ is given by

$$\pi^{\mathrm{G}}(\sigma) := \mu^L_{\beta,\gamma}(\sigma) = \frac{e^{-\beta H_\gamma(\sigma)}}{Z^\beta} \ . \tag{2.2.6}$$

where $\mu_{\beta,\gamma}(\sigma)$ denotes the probability of the configuration σ, in a volume $|\Lambda| = L$, at inverse temperature β. As usual, we indicate with Z^β the partition function, *i. e.* the normalization factor for (2.2.6)

$$Z^\beta = \sum_\sigma e^{-\beta H_\gamma(\sigma)} \ . \tag{2.2.7}$$

From now on, we will indicate the sum $\sum_{i=1}^L$ simply as $\sum_i$ for brevity.

Definition 2.2.1. We define the *empirical magnetization* on the volume B_i as

$$m_i := m_i^{\gamma}(\sigma) = \gamma \sum_{j \in B_i} \sigma_j = \sum_j J_\gamma(i,j)\ \sigma_j \tag{2.2.8}$$

where B_i is the block of sites of length $1/\gamma$ starting from the site $i+1$, *i. e.* $B_i = \{i+1, \ldots, i+1/\gamma\}$.

We can use definition (2.2.8) to rewrite the Hamiltonian (2.2.1) in the form

$$H_\gamma(\sigma) = -\sum_i \sigma_i m_i\ . \tag{2.2.9}$$

Before proceeding to present the dynamics we need to show a very interesting and useful fact about long range interactions on lattice with *periodic boundary conditions*.

2.3 The Global Balance Principle for non-reversible models

The well known *Detailed Balance Principle* is a very important concept in the study of dynamical processes and, in general, it marks the difference between *reversible* and *irreversible* systems. In statistical mechanics it is indeed a powerful tool to identify the stationary measure π of a Markov chain as the following brief theorem shows.

Theorem 2.3.1. Let P be the transition matrix of a homogeneous Markov chain and suppose there exists a distribution π such that $\pi_\sigma P_{\sigma,\tau} = \pi_\tau P_{\tau,\sigma}$ for all $\sigma, \tau \in S$. Then the Markov chain is said to be *reversible* and π is a stationary distribution of the chain and the dynamics.

Remark 2.3.1. Of course if the chain is *ergodic* π is *the* stationary distribution of the chain.

Proof. Suppose that π satisfies the conditions of the theorem. Then

$$\sum_\sigma \pi_\sigma P_{\sigma,\tau} = \sum_\sigma \pi_\tau P_{\tau,\sigma} = \pi_\tau \sum_\sigma P_{\tau,\sigma} = \pi_\tau \tag{2.3.1}$$

since $\sum_j P_{i,j} = 1$ by definition of transition matrix. Therefore, $\pi = \pi P$ so π is a stationary distribution. □

If a system does not satisfy the detailed balance there are non-zero fluxes in steady-state, it must have forces acting on it, hence it is said to be *time irreversible*. For such irreversible systems statistical mechanics is vastly more complicated but a weaker balance condition allows sometimes a straightforward computation of the stationary measure.
Since the dynamics we are going to study belongs to such class of systems, before giving the definitions we proceed showing this so called *Global Balance Principle* which we are able to prove for arbitrary range of interaction γ^{-1}, just imposing *periodic boundary conditions*.
Let's first present the general theorem.

Theorem 2.3.2 (Global Balance Principle). Let a Markov chain have the following transition probabilities

$$P_{\sigma\tau} = \frac{e^{-\beta H(\sigma,\tau)}}{\sum_\tau e^{-\beta H(\sigma,\tau)}} := \frac{e^{-\beta H(\sigma,\tau)}}{Z_\sigma} \ . \tag{2.3.2}$$

Then, under condition

$$\sum_\tau e^{-\beta H(\sigma,\tau)} = \sum_\tau e^{-\beta H(\tau,\sigma)} \ , \tag{2.3.3}$$

the probability distribution

$$\pi_\sigma = \frac{\sum_\tau e^{-\beta H(\sigma,\tau)}}{\sum_{\sigma\tau} e^{-\beta H(\sigma,\tau)}} = \frac{Z_\sigma}{\sum_\sigma Z_\sigma} := \frac{Z_\sigma}{Z^\beta} \tag{2.3.4}$$

is stationary.

Proof. By (2.3.3) and (2.3.4) we have

$$\begin{aligned} \sum_\sigma \pi_\sigma P_{\sigma,\tau} &= \sum_\sigma \frac{Z_\sigma}{Z^\beta} \frac{e^{-\beta H(\sigma,\tau)}}{Z_\sigma} \\ &= \frac{\sum_\sigma e^{-\beta H(\sigma,\tau)}}{Z^\beta} \\ &= \frac{\sum_\sigma e^{-\beta H(\tau,\sigma)}}{Z^\beta} = \frac{Z_\tau}{Z^\beta} = \pi_\tau \ . \end{aligned} \tag{2.3.5}$$

which is the definition of stationary distribution. Therefore the measure π is stationary. □

In order to prove the Global Balance Principle for the dynamics we will present in the next sections, we need to show an interesting, and very useful, fact regarding one-dimensional spin systems on a periodic lattice.

Proposition 2.3.1. Let $\Lambda = \{1 \dots L\}$ be a one-dimensional lattice with periodic boundary conditions and m_i and σ be as defined in Section 2.2. Then, for any function f,

$$\sum_{i\in\Lambda} f(m_i\sigma_i) = \sum_{i\in\Lambda} f(m_i\sigma_{i+1+1/\gamma}) \ . \tag{2.3.6}$$

Proof. Recalling the definition (2.2.8) we can define the *total magnetization* in the block B_i as

$$M_i := M_i(\sigma) = \frac{m_i(\sigma)}{\gamma} = \sum_{j\in B_i} \sigma_j \ , \quad B_i = \{i+1, \dots, i+1/\gamma\} \tag{2.3.7}$$

and notice that we have

$$M_i(\sigma) \in D \subset \mathbb{N} : D = \{-1/\gamma, -1/\gamma + 2, \dots, 1/\gamma\} \ . \tag{2.3.8}$$

The idea behind the proof of (2.3.6) is to show that for a fixed value of $M \in D$ the number of times we have $\sigma_i = +1$ is exactly equal to the number of times we have $\sigma_{i+1+1/\gamma} = +1$ and that, conversely, implies the same for $\sigma_i = \sigma_{i+1+1/\gamma} = -1$. In this way the positive and negative contributions to the r.h.s and the l.h.s. of (2.3.6) are equal $\forall\sigma \in S$, proving the equation.

For a fixed value of $M \in D$ we define

$$I_M = \{i \in \{1 \dots L\} \mid M_i(\sigma) = M\} \tag{2.3.9}$$

the set of points i such that $M_i(\sigma) = M$.
Then, define a series of families of points on Λ such that

$$I_1(M) = \begin{cases} \inf\{i_1 \in \Lambda : M_{i_1}(\sigma) = M\} & \text{if such } i_1 \text{ exists} \\ +\infty & \text{otherwise.} \end{cases} \tag{2.3.10}$$

If $I_1(M) < +\infty$ denote

$$I_2(M) = \begin{cases} \inf\{i_2 \in \Lambda,\ i_2 > i_1 : M_{i_2}(\sigma) = M\} & \text{if such } i_2 \text{ exists} \\ +\infty & \text{otherwise.} \end{cases} \tag{2.3.11}$$

Iterating the procedure we find a finite set $\mathcal{I}(M)$ of ordered points i on Λ such that $M_i(\sigma) = M$, *i. e.*

$$\mathcal{I}(M) = \{I_1(M),\ \dots,\ I_{k(M)}(M)\} \quad \text{with } k(M) \in [0, L]. \tag{2.3.12}$$

Now, let J be a permutation of the set $\mathcal{I}(M)$ defined as follows

i) if $|\mathcal{I}(M)| = 1 \to J\big(I_1(M)\big) = I_1(M)$

ii) if $|\mathcal{I}(M)| > 1$

$$J(I_l(M)) = \begin{cases} I_{k(M)}(M) & \text{for } l = 1, \\ I_{l-1}(M) & \text{for } l = 2,\ 3,\ \dots,\ k(M). \end{cases} \tag{2.3.13}$$

To simplify the notation from now on we will denote

$$J_l(M) = J(I_l(M)) \ . \tag{2.3.14}$$

Defining now

$$\overleftarrow{\sigma}_i = \sigma_i \ , \quad \overrightarrow{\sigma}_i = \sigma_{i+1+1/\gamma} \tag{2.3.15}$$

we can prove that for $i = I_l(M),\ j = J_l(M)$ we have

$$\overleftarrow{\sigma}_i = \overrightarrow{\sigma}_j \ . \tag{2.3.16}$$

Due to periodicity we clearly have that $M_{L+1} = M_1$, hence, we are sure that every time $M_{i-1} < M_i = M$ it will exist a site j such that $M = M_j > M_{j+1}$.

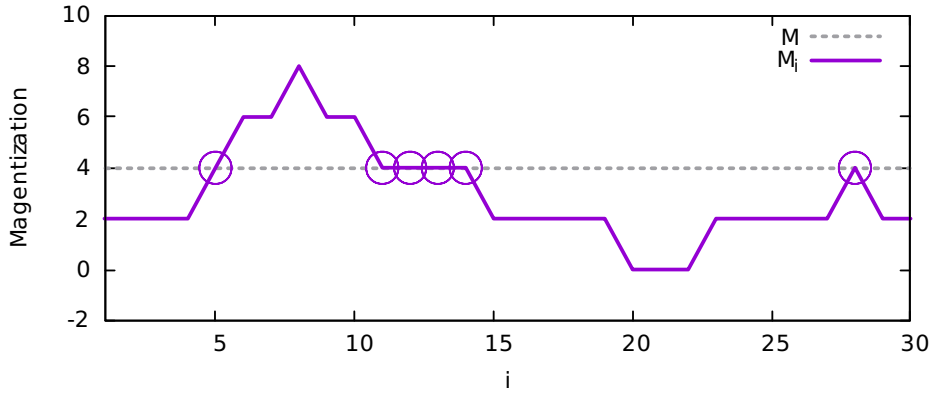

Figure 2.1: Example of absolute magnetization M_i where circles represent the family $\mathcal{I}(M)$ for $M = 4$ in the case that $\frac{1}{\gamma}$ is even.

Since

$$M_i = M_{i-1} - (\overleftarrow{\sigma}_i) + (\overrightarrow{\sigma}_i) \tag{2.3.17}$$

and we are in the case $M_{i-1} < M_i$, necessarily

$$\overleftarrow{\sigma}_i = -1 \tag{2.3.18}$$

Similarly, the relation

$$M_j = M_{j+1} + (\overleftarrow{\sigma}_j) - (\overrightarrow{\sigma}_j) \tag{2.3.19}$$

in the case $M_j > M_{j+1}$, yields to

$$\overrightarrow{\sigma}_j = -1 = \overleftarrow{\sigma}_i. \tag{2.3.20}$$

Repeating the same procedure for the case $M_{i-1} > M = M_i$ we obtain

$$\overleftarrow{\sigma}_i = +1 = \overrightarrow{\sigma}_j. \tag{2.3.21}$$

The case $M_{i+1} = M_i$ is trivial because it clearly implies

$$j = i - 1 \quad \rightarrow \quad \overrightarrow{\sigma}_j = \overleftarrow{\sigma}_i \tag{2.3.22}$$

and that proves (2.3.16).

Using relations (2.3.19) and (2.3.20), again with the same assumption $i = I_l(M)$, $j = J_l(M)$, it follows that for any function f

$$\sum_i f(M_i \overleftarrow{\sigma}_i) = \sum_M \sum_i f(M_i \overleftarrow{\sigma}_i) \mathbb{1}_{\{M_i = M\}} \ . \tag{2.3.23}$$

Fixing a value $M \in D$ we have

$$\begin{aligned}\sum_{i=1}^{L} f(M^{\overleftarrow{\sigma}_i})\mathbb{1}_{\{M_i=M\}} &= \sum_{l}^{k(M)} f(M^{\overleftarrow{\sigma}_{I_l(M)}})\mathbb{1}_{\{M_{I_l(M)}=M\}} \\ &= \sum_{l}^{k(M)} f(M^{\overrightarrow{\sigma}_{J_l(M)}})\mathbb{1}_{\{M_{J_l(M)}=M\}} \\ &= \sum_{j=1}^{L} f(M_j^{\overrightarrow{\sigma}_j})\mathbb{1}_{\{M_j=M\}} \ .\end{aligned} \tag{2.3.24}$$

Hence, we have that for any function f

$$\begin{aligned}\sum_i f(M_i^{\overleftarrow{\sigma}_i}) &= \sum_M \sum_i f(M_i^{\overleftarrow{\sigma}_i})\mathbb{1}_{\{M_i=M\}} \\ &= \sum_M \sum_i f(M_i^{\overrightarrow{\sigma}_i})\mathbb{1}_{\{M_i=M\}} = \sum_i f(M_i^{\overrightarrow{\sigma}_i}) \ .\end{aligned} \tag{2.3.25}$$

It's trivial that equation (2.3.25) is satisfied if we substitute M_i with m_i which completes the proof. □

In the following two sections we will present two irreversible dynamics, both introduced for the first time in this thesis. The first is an irreversible version of the Glauber dynamics, *i. e.* a single spin-flip Markov chain. Using Proposition 2.3.1 proved above we are able to show that its stationary measure is gibbsian. The second dynamics is a parallel one, and the rest of the thesis will discuss the (not yet completely solved) problem of the comparison between its stationary measure and the Gibbs measure. The identification of the stationary measure of such parallel dynamics is founded on the global balance principle and, again, Proposition 2.3.1.

2.4 Irreversible single spin-flip dynamics for the Kac-Ising model

We define an homogeneous Markov Chain based on the one dimensional Kac-Ising model with Hamiltonian (2.2.1). The *single spin-flip* dynamics works as follows:

1. choose a site $i \in \Lambda$ uniformly at random;

2. flip the spin σ_i with probability $e^{-2\beta[m_i(\sigma)\sigma_i + a]}$ with $a \geq 1$.

Note that the update rule we chose lets a spin i flip depending on the *local field* m_i generated by the spins at its *right*. Therefore, during the evolution of the Markov chain the time flow is clear and we will refer to it as an *irreversible* dynamics.

Remark 2.4.1. If in spite of definition (2.2.8) for $m_i^\gamma(\sigma)$ we use a *symmetrical* version of the empirical magnetization, *i. e.* such that $J_\gamma(i,j) = J_\gamma(j,i)$,

$$\bar{m}_i := \bar{m}_i^\gamma(\sigma) = \sum_j \bar{J}_\gamma(i,j)\sigma_j = \tfrac{\gamma}{2} \sum_j \sigma_j \mathbb{1}_{\{0<|j-i|\leq i+1/\gamma\}} \tag{2.4.1}$$

we get a *reversible* dynamics for which it's easy to see that the detailed balance condition with respect to the Gibbs measure (2.2.6) is satisfied.
In fact, calling $\sigma^{(i)}$ the configuration equal everywhere to σ except in the site i, *i. e.*

$$\sigma_k^{(i)} = \begin{cases} \sigma_k & \text{for } k \neq i \\ -\sigma_k & \text{for } k = i \ , \end{cases} \tag{2.4.2}$$

we can write the transition probabilities from configuration a $\sigma \in S$ to configuration a $\tau \in S$

$$P_{\sigma\tau} = \begin{cases} \frac{1}{|\Lambda|} e^{-2\beta(m_i\sigma_i + a)} & \text{if } \tau = \sigma^{(i)}, \\ 0 & \text{otherwise.} \end{cases} \tag{2.4.3}$$

Note that we clearly have $m_i^\gamma(\sigma) = m_i^\gamma(\sigma^{(i)})$ therefore

$$m_i^\gamma(\sigma)\sigma_i = -m_i^\gamma(\sigma^{(i)})\sigma_i^{(i)} \ . \tag{2.4.4}$$

Now, from (2.2.1)

$$\begin{aligned} H_\gamma(\sigma) &= -\sum_{j,k} \bar{J}_\gamma(j,k)\sigma_j\sigma_k \\ &= -\sum_{\substack{j,k \\ j,k\neq i}} \bar{J}_\gamma(j,k)\sigma_j\sigma_k - \sum_j \bar{J}_\gamma(j,i)\sigma_j\sigma_i - \sum_k \bar{J}_\gamma(i,k)\sigma_i\sigma_k \\ &= -\sum_{\substack{j,k \\ j,k\neq i}} \bar{J}_\gamma(j,k)\sigma_j\sigma_k - 2\bar{m}_i^\gamma(\sigma)\sigma_i \\ &= -\sum_{\substack{j,k \\ j,k\neq i}} \bar{J}_\gamma(j,k)\sigma_j^{(i)}\sigma_k^{(i)} + 2\bar{m}_i^\gamma(\sigma^{(i)})\sigma_i^{(i)} \\ &= H_\gamma(\sigma^{(i)}) + 4\bar{m}_i^\gamma(\sigma^{(i)})\sigma_i^{(i)} \end{aligned} \tag{2.4.5}$$

where we used the fact $\bar{J}_\gamma(i,j) = \bar{J}_\gamma(j,i)$.

Using relation (2.4.5) we can directly compute

$$\begin{aligned} \pi_\sigma^{\mathrm{G}} P_{\sigma\sigma^{(i)}} &= \frac{e^{-\beta H(\sigma)}}{Z_\beta}\frac{e^{-2\beta[\bar{m}_i^\gamma(\sigma)\sigma_i + a]}}{|\Lambda|} \\ &= \frac{1}{Z_\beta L} e^{-\beta[H(\sigma^{(i)}) + 4\bar{m}_i^\gamma(\sigma^{(i)})\sigma_i^{(i)} - 2\bar{m}_i^\gamma(\sigma^{(i)})\sigma_i^{(i)} + 2a]} \\ &= \frac{e^{-\beta H(\sigma^{(i)})}}{Z_\beta}\frac{e^{-2\beta[\bar{m}_i^\gamma(\sigma^{(i)})\sigma_i^{(i)} + a]}}{|\Lambda|} = \pi_{\sigma^{(i)}}^{\mathrm{G}} P_{\sigma^{(i)}\sigma} \end{aligned} \tag{2.4.6}$$

which is exactly the definition of the detailed balance condition given in Theorem 2.3.1. Hence, the Gibbs Measure π^{G} is the stationary measure of the reversible dynamics.

In the irreversible case we have in general that $J_\gamma(i,j) \neq J_\gamma(j,i)$ preventing the employment of the detail balance to compute the stationary measure of the irreversible dynamics. Nonetheless, calling

$$\overleftarrow{m}_i(\sigma) = \sum_j J_\gamma(j,i)\sigma_j \quad \text{and} \quad \overrightarrow{m}_i(\sigma) = \sum_k J_\gamma(i,k)\sigma_k \tag{2.4.7}$$

we can write

$$\begin{aligned} H_\gamma(\sigma) &= -\sum_{j,k} J_\gamma(j,k)\sigma_j\sigma_k \\ &= -\sum_{\substack{j,k \\ j,k\neq i}} J_\gamma(j,k)\sigma_j\sigma_k - \sum_j J_\gamma(j,i)\sigma_j\sigma_i - \sum_k J_\gamma(i,k)\sigma_i\sigma_k \\ &= -\sum_{\substack{j,k \\ j,k\neq i}} J_\gamma(j,k)\sigma_j\sigma_k - \overleftarrow{m}_i(\sigma)\sigma_i - \overrightarrow{m}_i(\sigma)\sigma_i \\ &= -\sum_{\substack{j,k \\ j,k\neq i}} J_\gamma(j,k)\sigma_j^{(i)}\sigma_k^{(i)} + \overleftarrow{m}_i(\sigma^{(i)})\sigma_i^{(i)} + \overrightarrow{m}_i(\sigma^{(i)})\sigma_i^{(i)} \\ &= H_\gamma(\sigma^{(i)}) + 2\overleftarrow{m}_i(\sigma^{(i)})\sigma_i^{(i)} + 2\overrightarrow{m}_i(\sigma^{(i)})\sigma_i^{(i)} \ . \end{aligned} \tag{2.4.8}$$

Applying directly the definition of stationary measure

$$\sum_\sigma \pi^{\mathrm{G}}_{\sigma^{(i)}} P_{\sigma^{(i)}\sigma} = \pi^{\mathrm{G}}_\sigma \tag{2.4.9}$$

we have that

$$\begin{aligned} \sum_\sigma \pi^{\mathrm{G}}_{\sigma^{(i)}} P_{\sigma^{(i)}\sigma} &= \sum_{i\in\Lambda} \frac{e^{-\beta H(\sigma^{(i)})}}{Z^\beta} P_{\sigma^{(i)}\sigma} + \frac{e^{-\beta H(\sigma)}}{Z^\beta}\left(1 - \sum_{i\in\Lambda} P_{\sigma\sigma^{(i)}}\right) \\ &= \sum_{i\in\Lambda} \frac{e^{-\beta\left(H(\sigma)+2\overleftarrow{m}_i(\sigma)\sigma_i+2\overrightarrow{m}_i(\sigma)\sigma_i\right)}}{Z^\beta} P_{\sigma^{(i)}\sigma} + \frac{e^{-\beta H(\sigma)}}{Z^\beta}\left(1 - \sum_{i\in\Lambda} P_{\sigma\sigma^{(i)}}\right) \\ &= \frac{e^{-\beta H(\sigma)}}{Z^\beta}\left[\sum_{i\in\Lambda} e^{-2\beta\left(\overleftarrow{m}_i(\sigma)\sigma_i+\overrightarrow{m}_i(\sigma)\sigma_i\right)} P_{\sigma^{(i)}\sigma} + 1 - \sum_{i\in\Lambda} P_{\sigma\sigma^{(i)}}\right] = \frac{e^{-\beta H(\sigma)}}{Z^\beta} \end{aligned} \tag{2.4.10}$$

where we used relation (2.4.8).
Therefore, to show that

$$\sum_{i\in\Lambda} e^{-2\beta\left(\overleftarrow{m}_i(\sigma)\sigma_i+\overrightarrow{m}_i(\sigma)\sigma_i\right)} P_{\sigma^{(i)}\sigma} = \sum_{i\in\Lambda} P_{\sigma\sigma^{(i)}} \tag{2.4.11}$$

we can substitute the transition probabilities $P_{\sigma^{(i)}\sigma}$ and $P_{\sigma\sigma^{(i)}}$ to get

$$\begin{aligned} &\sum_{i\in\Lambda} e^{-2\beta\left(\overleftarrow{m}_i(\sigma)\sigma_i+\overrightarrow{m}_i(\sigma)\sigma_i\right)} \frac{e^{-2\beta(\overrightarrow{m}_i(\sigma^{(i)})\sigma_i^{(i)}+a)}}{|\Lambda|} \\ &= \sum_{i\in\Lambda} \tfrac{1}{|\Lambda|} e^{-2\beta\left(\overleftarrow{m}_i(\sigma)\sigma_i+\overrightarrow{m}_i(\sigma)\sigma_i-\overrightarrow{m}_i(\sigma^{(i)})+a\right)} \\ &= \sum_{i\in\Lambda} \tfrac{1}{|\Lambda|} e^{-2\beta\left(\overleftarrow{m}_i(\sigma)\sigma_i+a\right)} = \sum_{i\in\Lambda} \tfrac{1}{|\Lambda|} e^{-2\beta(\overrightarrow{m}_i(\sigma)\sigma_i+a)} \end{aligned} \tag{2.4.12}$$

where we used formula (2.3.25) with the modification

$$\begin{aligned}\sum_i f(M_i\sigma_i) &= \gamma \sum_i f(\vec{m}_i(\sigma)\sigma_i) \\ &= \gamma \sum_i \left(\sum_j J_\gamma(i,j)\sigma_j\sigma_i \right) \\ &= \gamma \sum_j \left(\sum_i J_\gamma(i,j)\sigma_j\sigma_i \right) \\ &= \gamma \sum_i \left(\overleftarrow{m}_i(\sigma)\sigma_i \right) = \sum_i f(M_i\sigma_{i+1+1/\gamma}) \ .\end{aligned} \tag{2.4.13}$$

Therefore, also for the *irreversible* dynamics the stationary measure is Gibbsian.

Proven that the stationary distribution of both the dynamics is gibbsian, in Section 3.3 we present a numerical comparison between their mixing times. Measuring the *coalescence times*, *i. e.* the average number of iterations needed to coalesce for two Markov chains starting from opposite phases and evolving according to a suitable coupling, we are able to give an upper bound to the mixing time of the dynamics. We find that the ratio between the coalescence times of the reversible chain and the irreversible one is increasing with β and γ^{-1}, showing how the irreversible dynamics is faster to converge to equilibrium than its reversible counterpart.

2.5 Parallel Dynamics for Ising model with Kac potentials

As seen in Chapter 1, an interesting question in the study of particle systems, and in particular for the Ising model, is the implementation of a *parallel* dynamics. We can define an homogeneous Markov Chain based on the one dimensional Kac-Ising model *lifting* the Hamiltonian (2.2.1) to

$$H_\gamma(\sigma,\tau) = -H_0(\sigma,\tau) + \frac{Q(\sigma,\tau)}{\beta} \tag{2.5.1}$$

where

$$\begin{aligned} H_0(\sigma,\tau) &= \gamma \sum_i \sum_{j\in B_i} \sigma_i \tau_j \\ Q(\sigma,\tau) &= q \sum_i (1-\sigma_i\tau_i) \quad \text{with } q \geq 0. \end{aligned} \tag{2.5.2}$$

The transition probabilities from configuration a $\sigma \in S$ to configuration a $\tau \in S$ are defined as follows

$$P_{\sigma\tau} = \frac{e^{-\beta H_\gamma(\sigma,\tau)}}{\sum_\tau e^{-\beta H_\gamma(\sigma,\tau)}} := \frac{e^{-\beta H_\gamma(\sigma,\tau)}}{Z_\sigma} \ . \tag{2.5.3}$$

Observe that such probabilities can be factorized as a product of the probabilities of each component τ_i of the new configuration

$$P_{\sigma,\tau} = \Pi_{i=1}^{L} P\left(\tau_i|\sigma\right) \tag{2.5.4}$$

where

$$P(\tau_i|\sigma) = \frac{e^{[\beta\tau_i m_i - q(1-\sigma_i\tau_i)]}}{2e^{-q}\cosh\left(\beta m_i\sigma_i + q\right)} \ . \tag{2.5.5}$$

Therefore, this dynamics belongs to the family of Probabilistic Cellular Automata (PCA).

Differently from the *single spin-flip* dynamics, this new definition allows multiple sites to be updated in the same time-step. That's the reason to add in the Hamiltonian (2.5.1) the parameter q which represents an inertial term and models the tendency of the system to remain in its current state σ. In fact, as defined in (2.5.2), a strictly positive value of q increases the energy of a spin-flip, *i. e.* $\sigma_i \neq \tau_i$, de facto inhibiting the update of site i. In such a way we can control the average number of spin-flips in one iteration, adjusting the grade of *parallelism* of the dynamics.

Before facing the problem of finding the stationary measure of this PCA, in the next section we analyze a simpler case, the nearest neighbors interaction.

2.5.1 Nearest neighbors case

Proposition 2.5.1. The stationary measure of the dynamics (2.5.3) in the case $\gamma = 1$, *i. e.* every site i interacts only with his nearest neighbor site $i+1$, is the Gibbs measure, with a different temperature.

In other words we want, to show that, for $\gamma = 1$, for every value of the inverse temperature of the Gibbs measure β^{G} there exist couples of values β^{P} and q such that the stationary measure of the PCA dynamics π^{P} is exactly the Gibbs measure π^{G}.

Proof. Since for $\gamma = 1$

$$H_\gamma(\sigma) = \sum_{i,j} J_\gamma(i,j)\sigma_i\sigma_j = \sum_{i=1}^{L} \sigma_i\sigma_{i+1} \tag{2.5.6}$$

the Gibbs measure results to be

$$\pi^{\mathrm{G}}(\sigma) = \frac{1}{Z^{\mathrm{G}}} e^{-\beta^{\mathrm{G}} H_\gamma(\sigma)} = \frac{1}{Z^{\mathrm{G}}} \prod_{i=1}^{L} e^{\beta^{\mathrm{G}}(\sigma_i\sigma_{i+1})} = \frac{1}{Z^{\mathrm{G}}} e^{\beta^{\mathrm{G}} L} e^{-2J|\nu|} \tag{2.5.7}$$

where $|\nu|$ is the number of *contours*, *i. e.* in one dimension simply the number of pairs of adjacent spinf of different sign.
Therefore, we can write its partition function Z^{G} as follows

$$\begin{aligned} Z^{\mathrm{G}} = \sum_{\sigma} e^{-\beta^{\mathrm{G}} H(\sigma)} &= \sum_{\sigma} \prod_{i=1}^{L} e^{\beta^{\mathrm{G}}(\sigma_i\sigma_{i+1})} \\ &= \sum_{\sigma} \prod_{i=1}^{L} \cosh\left(\beta^{\mathrm{G}}(1 + \sigma_i\sigma_{i+1}\tanh\beta^{\mathrm{G}})\right) \\ &= 2^L \left[(\cosh\beta^{\mathrm{G}})^L + (\sinh\beta^{\mathrm{G}})^L\right] \end{aligned} \tag{2.5.8}$$

obtaining

$$\pi^{\mathrm{G}}(\sigma) = \frac{1}{2} \frac{e^{-2\beta^{\mathrm{G}}|\nu|}}{\sum\limits_{|\nu| \text{ even}} e^{-2\beta^{\mathrm{G}}|\nu|}} \ . \tag{2.5.9}$$

The Hamiltonian of the PCA dynamics in the case $\gamma = 1$ is

$$H_\gamma(\sigma,\tau)|_{\gamma=1} = H(\sigma,\tau) = -\sum_{i=1}^{L} \left(\sigma_i\tau_{i+1} - q(1 - \sigma_i\tau_i)\right) \tag{2.5.10}$$

and we can compute its stationary measure applying the global balance condition (2.3.3). In fact

$$\begin{aligned}\sum_{\tau} e^{-\beta^{\mathrm{P}} H(\sigma,\tau)} &= \sum_{\tau}\prod_{i} e^{\beta^{\mathrm{P}}(\sigma_i\tau_{i+1}-q+q\tau_i\sigma_i)} \\ &= e^{-qL\beta^{\mathrm{P}}}\sum_{\tau}\prod_{i} e^{\beta^{\mathrm{P}}(\sigma_{i-1}\tau_i+q\tau_i\sigma_i)} \\ &= 2^L e^{-qL\beta^{\mathrm{P}}}\prod_{i}\cosh\left(\beta^{\mathrm{P}}\sigma_{i-1}\sigma_i+q\right) \\ &= 2^L e^{-qL\beta^{\mathrm{P}}}\prod_{i}\cosh\left(\beta^{\mathrm{P}}\sigma_i\sigma_{i+1}+q\right) = \sum_{\tau} e^{-\beta^{\mathrm{P}} H(\tau,\sigma)}\end{aligned} \tag{2.5.11}$$

hence, the stationary measure π^{P} is

$$\begin{aligned}\pi^{\mathrm{P}}(\sigma) &= \frac{1}{Z^{\mathrm{P}}}\sum_{\tau} e^{-\beta^{\mathrm{P}} H(\sigma,\tau)} \\ &= \frac{1}{Z^{\mathrm{P}}}\sum_{\tau} e^{\beta^{\mathrm{P}}\sum_{i=1}^{L}(\sigma_i\tau_{i+1}+q\sigma_i\tau_i-q)} \\ &= \frac{1}{Z^{\mathrm{P}}}\sum_{\tau} e^{\beta^{\mathrm{P}}\sum_{i=1}^{L}(\sigma_{i-1}\tau_i+q\sigma_i\tau_i-q)} \\ &= \frac{2^L e^{-qL\beta^{\mathrm{P}}}}{Z^{\mathrm{P}}}\prod_{i=1}^{L}\cosh(\beta^{\mathrm{P}}\sigma_{i-1}\sigma_i+q) \\ &= \frac{2^L e^{-qL\beta^{\mathrm{P}}}}{Z^{\mathrm{P}}}\cosh(\beta^{\mathrm{P}}+q)^L\left(\frac{\cosh(\beta^{\mathrm{P}}-q)}{\cosh(\beta^{\mathrm{P}}+q)}\right)^{|\nu|}\end{aligned} \tag{2.5.12}$$

where, in the fourth row of the equation, we used the parity of the iperbolic cosine.
Writing the partition function Z^{P} as

$$Z^{\mathrm{P}} = 2^L e^{-qL\beta^{\mathrm{P}}}\sum_{|\nu|\ \text{even}}\cosh(\beta^{\mathrm{P}}+q)^L\left(\frac{\cosh(\beta^{\mathrm{P}}-q)}{\cosh(\beta^{\mathrm{P}}+q)}\right)^{|\nu|} \tag{2.5.13}$$

we have that

$$\pi^{\mathrm{P}}(\sigma) = \frac{1}{2}\frac{\left(\frac{\cosh(\beta^{\mathrm{P}}-q)}{\cosh(\beta^{\mathrm{P}}+q)}\right)^{|\nu|}}{\sum_{\gamma}\left(\frac{\cosh(\beta^{\mathrm{P}}-q)}{\cosh(J+q)}\right)^{|\nu|}}\ . \tag{2.5.14}$$

Imposing $\pi^{\mathrm{P}}(\sigma) = \pi^{\mathrm{G}}(\sigma)$ we have that

$$\pi^{\mathrm{G}}(\sigma) = \frac{1}{2}\frac{e^{-2\beta^{\mathrm{G}}|\nu|}}{\sum_{|\nu|\ \text{even}} e^{-2\beta^{\mathrm{G}}|\nu|}} = \frac{1}{2}\frac{\left(\frac{\cosh(\beta^{\mathrm{P}}-q)}{\cosh(\beta^{\mathrm{P}}+q)}\right)^{|\nu|}}{\sum_{|\nu|\ \text{even}}\left(\frac{\cosh(\beta^{\mathrm{P}}-q)}{\cosh(\beta^{\mathrm{P}}+q)}\right)^{|\nu|}} = \pi^{\mathrm{P}}(\sigma)\ , \tag{2.5.15}$$

therefore, calling $b = \tanh(q)$,

$$\begin{aligned} e^{-2\beta^{\mathrm{G}}} &= \left(\frac{\cosh(\beta^{\mathrm{P}} - q)}{\cosh(\beta^{\mathrm{P}} + q)}\right) = \frac{1 - \tanh\beta^{\mathrm{P}} b}{1 + \tanh\beta^{\mathrm{P}} b} \\ &= \frac{1 - b\frac{\sinh\beta^{\mathrm{P}}}{\cosh\beta^{\mathrm{P}}}}{1 + b\frac{\sinh\beta^{\mathrm{P}}}{\cosh\beta^{\mathrm{P}}}} = \frac{\cosh\beta^{\mathrm{P}} - b\sinh\beta^{\mathrm{P}}}{\cosh\beta^{\mathrm{P}} + b\sinh\beta^{\mathrm{P}}} \\ &= \frac{e^{\beta^{\mathrm{P}}} + e^{-\beta^{\mathrm{P}}} - be^{\beta^{\mathrm{P}}} + be^{-\beta^{\mathrm{P}}}}{e^{\beta^{\mathrm{P}}} + e^{-\beta^{\mathrm{P}}} + be^{\beta^{\mathrm{P}}} - be^{-\beta^{\mathrm{P}}}} \\ &= \frac{(1-b)e^{\beta^{\mathrm{P}}} + (1+b)e^{-\beta^{\mathrm{P}}}}{(1+b)e^{\beta^{\mathrm{P}}} + (1-b)e^{-\beta^{\mathrm{P}}}} \\ &= \frac{(1-b) + (1+b)e^{-2\beta^{\mathrm{P}}}}{(1+b) + (1-b)e^{-2\beta^{\mathrm{P}}}} \ . \end{aligned} \tag{2.5.16}$$

Rearranging the terms we have

$$\begin{aligned} (1-b) + (1+b)e^{-2\beta^{\mathrm{P}}} &= e^{-2\beta^{\mathrm{G}}}\left((1+b) + (1-b)e^{-2\beta^{\mathrm{P}}}\right) \\ e^{-2\beta^{\mathrm{P}}}\left((1+b) - e^{-2\beta^{\mathrm{G}}}(1+b)\right) &= e^{-2\beta^{\mathrm{G}}}(1+b) - (1-b) \end{aligned} \tag{2.5.17}$$

obtainig the following relation between β^{P} and β^{G}

$$\begin{aligned} e^{-2\beta^{\mathrm{P}}} &= \frac{e^{-2\beta^{\mathrm{G}}}(1+b) - (1-b)}{(1+b) - e^{-2\beta^{\mathrm{G}}}(1+b)} \\ &= e^{-2\beta^{\mathrm{G}}}\frac{1 + b - (1-b)e^{2\beta^{\mathrm{G}}}}{1 + b - (1-b)e^{-2\beta^{\mathrm{G}}}} \end{aligned} \tag{2.5.18}$$

□

From (2.5.18) it's clear that for every β^{G} it exist a surface (β^{P}, q), a curve in this case, such that $\pi^{\mathrm{G}} = \pi^{\mathrm{P}}$ and since $0 < (1-b) < 1\ \forall q > 0$ the last fraction in (2.5.18) is less than 1 implying that $\beta^{\mathrm{P}} > \beta^{\mathrm{G}}$. Furthermore, being $e^{-2\beta^{\mathrm{P}}}$ positive, clearly $(1+b) > (1-b)e^{2\beta^{\mathrm{G}}}$, thus, for big values of β^{G}, *i. e.* at low temperature, $b = \tanh(q)$ must be close to 1. Therefore the curve (β^{P}, q) is shorter when β^{G} is big and longer when β^{G} is small.

2.6 Gibbs measure

To identify the stationary measure of the PCA dynamics presented in Section 2.5 in the general case $\gamma < 1$ we have, again, to resort to the Global Balance Principle. To show that the dynamics fulfills the conditions of Theorem 2.3.2 we have to show that

$$\sum_{\tau} e^{-\beta H(\sigma,\tau)} = \sum_{\tau} e^{-\beta H(\tau,\sigma)} \ . \tag{2.6.1}$$

Writing both expressions as

$$\begin{cases} \sum_{\tau} e^{-\beta H(\tau,\sigma)} = 2^L e^{-qL\beta} \prod_{i=1}^{L} \cosh(\beta m_i \sigma_i + q) \\ \sum_{\tau} e^{-\beta H(\sigma,\tau)} = 2^L e^{-qL\beta} \prod_{i=1}^{L} \cosh(\beta m_i \sigma_{i+1+\frac{1}{\gamma}} + q) \end{cases} \tag{2.6.2}$$

we see that it's sufficient to prove that

$$\prod_{i=1}^{L} \cosh(\beta m_i \sigma_i + q) = \prod_{i=1}^{L} \cosh(\beta m_i \sigma_{i+1+\frac{1}{\gamma}} + q) \ . \tag{2.6.3}$$

That can be easily done using formula (2.3.25) from Proposition 2.3.1 and choosing the function f as follows

$$f = \cosh\left(\beta\gamma M_i \sigma_i + q\right) \ . \tag{2.6.4}$$

The expression of stationary measure of the PCA is therefore the one in (2.3.4), *i. e.*

$$\pi^{\mathrm{P}}(\sigma) = \frac{w_\sigma^{\mathrm{P}}}{\sum_\sigma w_\sigma^{\mathrm{P}}} = \frac{w_\sigma^{\mathrm{P}}}{Z^{\mathrm{P}}} \tag{2.6.5}$$

where we have defined the PCA *weight* of the configuration σ

$$w_\sigma^{\mathrm{P}} = \sum_{\tau} e^{-\beta H_\gamma(\sigma,\tau)} \ . \tag{2.6.6}$$

Recalling the classical Ising model presented in Section 2.2 it is a standard task to derive its Gibbs Measure, which we recall to be defined as

$$\pi^{\mathrm{G}}(\sigma) = \frac{w_\sigma^{\mathrm{G}}}{\sum_\sigma w_\sigma^{\mathrm{G}}} = \frac{w_\sigma^{\mathrm{G}}}{Z^{\mathrm{G}}} \tag{2.6.7}$$

where we have defined the gibbsian *weight* of the configuration σ as follows

$$w_\sigma^{\mathrm{G}} = e^{-\beta H_\gamma(\sigma)} = e^{\beta \sum_i \sigma_i m_i} \ . \tag{2.6.8}$$

To show the relation between the Gibbs measure π^{G} and the PCA's stationary measure π^{P} we follow a procedure already used in [15].

Calling I the subset such that $I = \{i \in V : \sigma_i \neq \tau_i\}$ we have

$$\begin{aligned} w^{\mathrm{P}}_{\sigma} &= \sum_{\tau} e^{-\beta H(\sigma,\tau)} = \sum_{\tau} e^{\beta \sum_i \tau_i m_i - q \sum_i (1-\sigma_i\tau_i)} \\ &= \sum_{I \subset V} e^{\beta \sum_i \sigma_i m_i - 2\beta \sum_{i\in I} \sigma_i m_i - 2q|I|} \\ &= w^{\mathrm{G}}_{\sigma} \prod_{i\in V} (1+\delta\phi_i) = w^{\mathrm{G}}_{\sigma} f(\sigma) \end{aligned} \tag{2.6.9}$$

where $\delta = e^{-2q}$ and

$$\phi_i \equiv e^{-2\beta\sigma_i m_i} \tag{2.6.10}$$

and $f(\sigma)$ is the function

$$f(\sigma) \equiv \prod_{i\in V} (1+\delta\phi_i) \ . \tag{2.6.11}$$

Denoting now

$$Z^{\mathrm{P}} = \sum_{\sigma} w^{\mathrm{P}}_{\sigma} \tag{2.6.12}$$

and computing

$$\begin{aligned} \pi^{\mathrm{P}}(\sigma) &= \frac{w^{\mathrm{P}}_{\sigma}}{\sum_\sigma w^{\mathrm{P}}_{\sigma}} = \frac{w^{\mathrm{G}}_{\sigma} f(\sigma)}{\sum_\sigma w^{\mathrm{G}}_{\sigma} f(\sigma)} \\ &= \frac{w^{\mathrm{G}}_{\sigma} f(\sigma)}{\sum_\sigma w^{\mathrm{G}}_{\sigma}} \frac{\sum_\sigma w^{\mathrm{G}}_{\sigma}}{\sum_\sigma w^{\mathrm{G}}_{\sigma} f(\sigma)} = \frac{\pi^{\mathrm{G}}(\sigma) f(\sigma)}{\pi^{\mathrm{G}}(f)} \end{aligned} \tag{2.6.13}$$

we obtain the following relation between the two stationary measures

$$\pi^{\mathrm{P}}(\sigma) = \pi^{\mathrm{G}}(\sigma) \frac{f(\sigma)}{\pi^{\mathrm{G}}(f)} \ . \tag{2.6.14}$$

Due to the form of expression (2.6.11) we can easily show the convergence of π^{P} to π^{G} under the condition

$$\delta = e^{-2q} < \frac{1}{L} \ . \tag{2.6.15}$$

Defining

$$\phi_{min} = \inf_{i\in\Lambda}\{\phi_i\} \quad \text{and} \quad \phi_{max} = \sup_{i\in\Lambda}\{\phi_i\} \tag{2.6.16}$$

we have

$$\prod_{i=1}^{L}(1+\delta\phi_{min}) \leq \prod_{i=1}^{L}(1+\delta\phi) \leq \prod_{i=1}^{L}(1+\delta\phi_{max}) \tag{2.6.17}$$

which implies

$$(1+\delta\phi_{min})^L \leq (1+\delta\phi)^L \leq (1+\delta\phi_{max})^L \ . \tag{2.6.18}$$

In the limit $L \to \infty$ we have

$$e^{\delta\phi_{min}L} \leq e^{\delta\phi L} \leq e^{\delta\phi_{max}L} \tag{2.6.19}$$

and condition (2.6.15) on δ guarantees that $\delta L \to 0$ so the extremes of the expression force $f(\sigma)$ to be equal to 1 which, due to equation (2.6.14), proves $\pi^{\mathrm{P}} \to \pi^{\mathrm{G}}$.
Condition (2.6.15) is however a strong requirement for the parallel dynamics because recalling the transition probabilities (2.5.5), the condition

$$\delta = e^{-2q} \leq \frac{1}{L^{1+\varepsilon}} \tag{2.6.20}$$

for some $\varepsilon > 0$, results in

$$P(\tau_i \neq \sigma_i) = \frac{e^{-\beta\gamma\sum_{j\in B_i}\sigma_i\tau_j - 2q}}{Z_\sigma} \leq \frac{e^{\beta-2q}}{Z_\sigma} \leq \frac{e^{\beta}}{Z_\sigma}\frac{1}{L^{1+\varepsilon}} \ . \tag{2.6.21}$$

In the single iteration from σ to τ the probability to have a different spin in a specific site i is less than the inverse of the volume size L. Hence the PCA becomes, on average, equivalent to a *single spin-flip* dynamics.

2.7 High temperature via Föllmer covariance estimates

In order to obtain the convergence of the PCA stationary measure to the Gibbs measure in a truly parallel dynamics we will follow the approach taken in the main theorem of [15].
The idea of the proof is to control the decay of correlations of the family of functions ϕ_i, defined in (2.6.10), using the well-known Dobrushin condition for uniqueness of phase

$$\sup_i \sum_j \tanh\left(2|J_{i,j}|\right) < 1 \ , \tag{2.7.1}$$

provided that $\delta = e^{-2q}$ is such that

$$\lim_{L\to\infty} \delta^2 L = 0 \ . \tag{2.7.2}$$

In such a way the probability of a spin-flip in a site i is

$$P(\tau_i \neq \sigma_i) = \frac{e^{-\beta\gamma\sum_{j\in B_i}\sigma_i\tau_j - 2q}}{Z_\sigma} < \frac{e^{\beta-2q}}{Z_\sigma} < \frac{1}{Z_\sigma}\frac{e^\beta}{\sqrt{L}} \ , \tag{2.7.3}$$

hence, the average number of spins updated in each time step is of order $\sqrt{L}$, in opposition to the dynamics implied by the stronger condition (2.6.20) which results to be essentially sequential.

The original statement of the main theorem in [15] reads as follows

Theorem 2.7.1. For any $q \geq 0$ let $\delta = e^{-2q}$. Suppose:

(a) $\delta = \delta(L)$ is such that $\lim_{L\to\infty} \delta^2 L = 0$;

(b) there exists δ_0 such that

$$\sup_\Lambda \sup_{\delta\in[0,\delta_0]} \frac{1}{L}\mathrm{Var}_\pi\left[\sum_{i\in\Lambda}\frac{\phi_i}{1+\phi_i}\right] < \infty \tag{2.7.4}$$

for $\pi = \frac{f(\sigma)}{\pi^{\mathrm{G}}(f)}$ and $\pi = \frac{f(\sigma)^2}{\pi^{\mathrm{G}}(f^2)}$.

Then

$$\lim_{L\to\infty} \|\pi^{\mathrm{P}} - \pi^{\mathrm{G}}\|_{TV} = 0 \tag{2.7.5}$$

where the *Total Variation Distance* between the PCA's stationary measure and the Gibbsian one is defined as

$$\|\pi^{\mathrm{P}} - \pi^{\mathrm{G}}\|_{TV} \equiv \tfrac{1}{2}\sum_\sigma \left|\pi^{\mathrm{P}}(\sigma) - \pi^{\mathrm{G}}(\sigma)\right| . \tag{2.7.6}$$

Using relation (2.6.14) we can derive that

$$\begin{aligned}\|\pi^{\mathrm{P}} - \pi^{\mathrm{G}}\|_{TV} &= \tfrac{1}{2}\sum_{\sigma} \pi^{\mathrm{G}}(\sigma)\left|\frac{f(\sigma)}{\pi^{\mathrm{G}}(f)} - 1\right| \\ &= \tfrac{1}{2}\sum_{\sigma} \frac{w^{\mathrm{G}}(\sigma)}{Z^{\mathrm{G}}}\left|\frac{f(\sigma)}{\pi^{\mathrm{G}}(f)} - 1\right| \\ &= \tfrac{1}{2}\pi^{\mathrm{G}}\left(\left|\frac{f(\sigma)}{\pi^{\mathrm{G}}(f)} - 1\right|\right)\end{aligned} \tag{2.7.7}$$

and now, defining

$$\Delta(\delta) = \frac{\pi_G(f^2)}{(\pi_G(f))^2} - 1 \tag{2.7.8}$$

we have, by Cauchy-Schwarz inequality,

$$\begin{aligned}\pi^{\mathrm{G}}\left(\left|\frac{f(\sigma)}{\pi^{\mathrm{G}}(f)} - 1\right|\right) &\le \sqrt{\pi^{\mathrm{G}}\left(\left(\frac{f(\sigma)}{\pi^{\mathrm{G}}(f)} - 1\right)^2\right)} \\ &= \sqrt{\pi^{\mathrm{G}}\left(\frac{(f(\sigma) - \pi^{\mathrm{G}}(f))^2}{(\pi^{\mathrm{G}}(f))^2}\right)} \\ &= \sqrt{\frac{\pi^{\mathrm{G}}(f^2)}{\pi^{\mathrm{G}}(f)^2} - 1} = \sqrt{\Delta(\delta)}\ .\end{aligned} \tag{2.7.9}$$

To prove the theorem under condition (a), we just need to control $\Delta(\delta)$ around $\delta = 0$ up to the second order showing that

$$\Delta(\delta) = \frac{1}{L}\log \pi^{\mathrm{G}}(f^2) - \frac{2}{L}\log \pi^{\mathrm{G}}(f) = O(\delta^2)\ . \tag{2.7.10}$$

Let us define

$$\tilde{\pi}(\sigma) = \pi^{\mathrm{G}}(\sigma)\frac{f^2}{\pi^{\mathrm{G}}(f^2)} \tag{2.7.11}$$

and, recalling definition (2.6.11), rewrite $f(\sigma)$ as

$$f(\sigma) = \exp\left[\sum_{i\in\Lambda} \log\left(1 + \delta\phi_i(\sigma)\right)\right]\ . \tag{2.7.12}$$

Using these expressions we can explicitly compute

$$\frac{d}{d\delta}\log \pi^{\mathrm{G}}(f) = \pi^{\mathrm{P}}\left[\sum_{i\in\Lambda}\frac{\phi_i}{1 + \delta\phi_i}\right]\ , \tag{2.7.13}$$

$$\frac{d}{d\delta}\log\pi^{\mathrm{G}}(f^2) = 2\tilde{\pi}\left[\sum_{i\in\Lambda}\frac{\phi_i}{1+\delta\phi_i}\right] , \tag{2.7.14}$$

$$\frac{d^2}{d^2\delta}\log\pi^{\mathrm{G}}(f) = -\pi^{\mathrm{P}}\left[\sum_{i\in\Lambda}\left(\frac{\phi_i}{1+\delta\phi_i}\right)^2\right] + \mathrm{Var}_{\pi^{\mathrm{P}}}\left[\frac{\phi_i}{1+\delta\phi_i}\right] , \tag{2.7.15}$$

and

$$\frac{d^2}{d^2\delta}\log\pi^{\mathrm{G}}(f^2) = -2\tilde{\pi}\left[\sum_{i\in\Lambda}\left(\frac{\phi_i}{1+\delta\phi_i}\right)^2\right] + 4\mathrm{Var}_{\tilde{\pi}}\left[\frac{\phi_i}{1+\delta\phi_i}\right] . \tag{2.7.16}$$

Since the first order expansion of $\Delta(\delta)$ in $\delta = 0$ presents an explicit cancellation, due to the fact that $\pi^{\mathrm{G}} = \pi^{\mathrm{P}} = \tilde{\pi}$ for $\delta = 0$, to prove (2.7.10) it is enough to show that the following holds

$$\sup_{\Lambda}\sup_{\delta}\frac{1}{L}\left(\left|\frac{d^2}{d^2\delta}\log\pi^{\mathrm{G}}(f)\right| + \left|\frac{d^2}{d^2\delta}\log\pi^{\mathrm{G}}(f^2)\right|\right) < +\infty . \tag{2.7.17}$$

What it is to be shown is that the *Dobrushin uniqueness condition* (2.7.1) guarantees that assumption (b) in Theorem 2.7.1 holds which, in turn, implies (2.7.17). That is achieved using the main result of Föllmer's paper [21], see also Kunsch's work [36], which gives an estimate for the covariance of the Gibbs measure under very general conditions, among which (2.7.1).

2.7.1 Föllmer covariance estimate

Suppose the following

- μ is a probability measure on a product space $E = S^I$ and we know for all points $k \in I$ the conditional distribution $\mu_k(dx_k|x)$;
- C is the so called *Dobrushin interaction matrix* with elements

  $$C_{ik} = \sup\left\{\tfrac{1}{2}\|\mu_k(\cdot|x) - \mu_k(\cdot|y)\|_1 : x = y \text{ off } \{i\}\right\} \tag{2.7.18}$$

  and assume the following condition holds

  $$\alpha = \sup_k \sum_i C_{ik} < 1 ; \tag{2.7.19}$$

- D is the matrix with elements $D_{ik} = \sum_{n=0}^{\infty} C^n$;

- $\rho_i(f)$ is the so called *oscillation* of f in the point i defined as

$$\rho_i(f) = \sup\Big\{|f(x) - f(y)| : x = y \text{ off } \{i\}\Big\} \; ; \tag{2.7.20}$$

Then, Föllmer's Theorem can be expressed as follows.

Theorem 2.7.2. Under condition (2.7.19), the covariance of any two functions f and g in $C(E)$ with respect to μ satisfies

$$\big|\mathrm{Cov}_\mu(f,g)\big| \leq \tfrac{1}{4}\sum_{i,k}\rho_i(f)D_{ik}\rho_k(g) \; . \tag{2.7.21}$$

See Appendix A for the proof.

2.7.2 Proof of Theorem 2.7.1

In order to apply Föllmer Theorem we have to show that Dobrushin uniqueness condition (2.7.1) implies condition (2.7.19).

Proposition 2.7.1. Let C_{ij} be the elements of the Dobrushin interaction matrix for the measure π, as defined in (2.7.18), and $J_{i,j}$ the potential between sites i and j. Then

$$C_{ij} \leq \tanh(2|J_{i,j}|) + \tfrac{1}{2}\rho_j(\psi_{i,\delta}) \tag{2.7.22}$$

where $\psi_{i,\delta}$ is defined by

$$\psi_{i,\delta}(\sigma) = \tfrac{1}{2}\log\frac{1+\delta e^{-2h_i(\sigma)}}{1+\delta e^{2h_i(\sigma)}} + \tfrac{1}{2}\sum_{l>0}\log\frac{1+\delta e^{-2J_{i,l}\sigma_l - 2\sigma_l h_{i,l}(\sigma)}}{1+\delta e^{2J_{i,l}\sigma_l - 2\sigma_l h_{i,l}(\sigma)}} \tag{2.7.23}$$

and

$$h_i(\sigma) = \sum_j J_{ij}\sigma_j \; , \; h_{i,l}(\sigma) = \beta\sum_{j\neq l} J_{i,j}\sigma_j \; . \tag{2.7.24}$$

Proof. Consider the simple case $i = 0$ and $\pi = \pi^{\mathrm{P}}$, the proof for $\pi = \tilde{\pi}$ is similar. We write

$$H_i = \log(1 + \delta\phi_i) \tag{2.7.25}$$

so that

$$\pi^{\mathrm{P}}(\sigma) = \frac{1}{Z^{\mathrm{P}}}\exp\left[\sum_{i,j} J_{i,j}\sigma_i\sigma_j + \sum_i H_i(\sigma)\right] \; . \tag{2.7.26}$$

Note that, calling $\sigma_{\setminus i}$ the configuration σ without the point i, we can write it as

$$\sum_{i,j} J_{i,j}\sigma_i\sigma_j = 2\sigma_0 h_0(\sigma) + C_1(\sigma_{\setminus 0}) \tag{2.7.27}$$

where $C_1(\sigma_{\setminus 0})$ denotes all remaining terms which do not depend on σ_0. In such a way we have isolated the *odd* terms, which depend on the sign σ_0, from its *even* ones $C_1(\sigma_{\setminus 0})$.
Similarly

$$\begin{aligned} H_0(\sigma) &= \log(1+\delta e^{2\sigma_0 h_0(\sigma)}) \\ &= \tfrac{1}{2}\sigma_0 \log\frac{1+\delta e^{-2h_0(\sigma)}}{1+\delta e^{2h_0(\sigma)}} + C_2(\sigma_{\setminus 0}) \end{aligned} \tag{2.7.28}$$

and for all $l \neq 0$

$$\begin{aligned} H_l(\sigma) &= \log\left(1+\delta e^{-2\sigma_l \sum_j J_{l,j}\sigma_j}\right) \\ &= \log\left(1+\delta e^{-2J_{0,l}\sigma_0\sigma_l - 2\sigma_l h_{0,l}(\sigma)}\right) \\ &= \tfrac{1}{2}\sigma_0 \log\frac{1+\delta e^{-2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}}{1+\delta e^{2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}} + C_3(\sigma_{\setminus 0})\ . \end{aligned} \tag{2.7.29}$$

It follows that

$$\pi^{\mathrm{P}}(\sigma_0 = 1|\sigma_{\setminus 0}) = \frac{e^{2h_0(\sigma)+\psi_{0,\delta}}}{2\cosh(2h_0(\sigma)+\psi_{0,\delta})}\ . \tag{2.7.30}$$

Writing, ψ_δ for $\psi_{0,\delta}$ and $\sigma^{(j)}$ according to (2.4.2), we have

$$2h_0(\sigma)+\psi_\delta(\sigma) - \big(2h_0(\sigma^{(j)})+\psi_\delta(\sigma^{(j)})\big) = 4J_{0,j} + \psi_\delta(\sigma) - \psi_\delta(\sigma^{(j)})\ . \tag{2.7.31}$$

Setting now $x = -2h_0(\sigma)\psi_\delta(\sigma)$ and $y = 4J_{0,j} + \psi_\delta(\sigma) - \psi_\delta(\sigma^{(j)})$ we call

$$\begin{aligned} g_y(x) :&= \pi^{\mathrm{P}}(\sigma_0 = 1|\sigma_{\setminus 0}) - \pi^{\mathrm{P}}(\sigma_0 = 1|\sigma^{(j)}_{\setminus 0}) \\ &= \frac{e^{-x}}{2\cosh(x)} - \frac{e^{-x-y}}{2\cosh(x+y)}\ . \end{aligned} \tag{2.7.32}$$

Unless $y = 0$ (which gives $g_y = 0$), the derivative $(g_y^2)'$ vanishes only at $x = -y/2$, where g_y^2 attains its absolute maximum $\tanh^2(y/2)$.
This yields

$$|\pi^{\mathrm{P}}(\sigma_0 = 1|\sigma_{\setminus 0}) - \pi^{\mathrm{P}}(\sigma_0 = 1|\sigma^{(j)}_{\setminus 0})| \leq \tanh\left(2|J_{0,j}| + \tfrac{1}{2}|\psi_\delta(\sigma) - \psi_\delta(\sigma^{(j)})|\right)\ . \tag{2.7.33}$$

Since, for every $a, b \geq 0$, $\tanh(a+b) \leq \tanh(a)+b$ we have that the conclusion of the Proposition 2.7.1 follows. □

To complete the proof of Theorem 2.7.1 we need to prove the following lemma.

Lemma 2.7.1. The quantity $\psi_{i,\delta}$, as defined in (2.7.23), is such that

$$\sup_i \sum_j \rho_j(\psi_{i,\delta}) = O(\delta) \quad \text{as } \delta \to 0 \ . \tag{2.7.34}$$

Proof. Set $i = 0$ and $\psi_{0,\delta} = \psi_\delta$. The estimate for a generic i is similar. Ignoring an irrelevant factor 2

$$\begin{aligned}\rho_j(\psi_\delta) \le \rho_j\left(\log\frac{1+\delta e^{-2h_0(\delta)}}{1+\delta e^{2h_0(\delta)}}\right) + \rho_j\left(\log\frac{1+\delta e^{-2J_{0,j}\sigma_j - 2\sigma_j h_{0,j}(\sigma)}}{1+\delta e^{2J_{0,j}\sigma_j - 2\sigma_j h_{0,j}(\sigma)}}\right) \\ + \sum_{l\neq 0,j}\rho_j\left(\log\frac{1+\delta e^{-2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}}{1+\delta e^{2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}}\right) \ .\end{aligned} \tag{2.7.35}$$

The main difficulty comes from the third term, and we only deal with it, *i. e.* we show that

$$\sum_j \sum_{l\neq 0,j} \rho_j\left(\log\frac{1+\delta e^{-2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}}{1+\delta e^{2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}}\right) = O(\delta) \ . \tag{2.7.36}$$

Set

$$\begin{aligned}C_l(\delta) :&= \log\frac{1+\delta e^{-2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}}{1+\delta e^{2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}} \\ &= \log\left(1 - 2\delta\frac{\sinh(2J_{0,l}\sigma_l)e^{-2\sigma_l h_{0,l}(\sigma)}}{1+\delta e^{2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}}\right) \ .\end{aligned} \tag{2.7.37}$$

It is not restrictive to assume that δ is small so that

$$2\delta\frac{\sinh(2|J_{0,l}|)e^{-2\sigma_l h_{0,l}(\sigma)}}{1+\delta e^{2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}} < \tfrac{1}{2} \ . \tag{2.7.38}$$

Since, on $(-\frac{1}{2}, \frac{1}{2})$ the map $x \to \log(1-x)$ has Lipschitz constant 2, we have

$$\begin{aligned}|C_l(\delta) - C_l(\delta^j)| &\le 4\delta\sinh(2|J_{0,l}|)\left|\frac{e^{-2\sigma_l h_{0,l}(\sigma^{(j)})}}{1+\delta e^{2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma^{(j)})}} - \frac{e^{-2\sigma_l h_{0,l}(\sigma)}}{1+\delta e^{2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}}\right| \\ &\le 4\delta\sinh(2|J_{0,l}|)\left|e^{-2\sigma_l h_{0,l}(\sigma^{(j)})} - e^{-2\sigma_l h_{0,l}(\sigma)}\right| \\ &\le 4\delta e^{2J}\sinh(2|J_{0,l}|)\left|h_{0,l}(\sigma^{(j)}) - h_{0,l}(\sigma)\right| \\ &\le 4\delta e^{4J}|J_{0,l}||J_{j,l}|\end{aligned} \tag{2.7.39}$$

where we have also used the facts that the map $x \to \frac{x}{1+ax}$ has Lipschitz constant 1 for $x > 0$ and $a > 0$, that $|e^x - e^y| \le e^{\max(|x|,|y|)}|x-y|$ and that $\sinh(2|J_{0,l}|) \le e^{2J}|J_{0,l}|$.

It follows that

$$\sum_j \sum_{l\neq 0,j} \rho_j \left(\log \frac{1+\delta e^{-2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}}{1+\delta e^{2J_{0,l}\sigma_l - 2\sigma_l h_{0,l}(\sigma)}} \right) \leq 4\delta e^{4J} J^2 = O(\delta) \ . \tag{2.7.40}$$

□

At this point, choosing $\mu = \pi$, $f = \frac{\phi_i}{1+\phi_i}$ and $g = \frac{\phi_j}{1+\phi_j}$ we can use Föllmer's Theorem 2.7.2 to compute

$$\begin{aligned} \frac{1}{L}\mathrm{Var}_\pi \left[\sum_{i\in\Lambda} \frac{\phi_i}{1+\phi_i} \right] &= \frac{1}{L} \sum_{i,j\in\Lambda} \mathrm{Cov}_\pi \left(\frac{\phi_i}{1+\phi_i}, \frac{\phi_j}{1+\phi_j} \right) \\ &\leq \frac{1}{L} \sum_{i,j\in\Lambda} \sum_{h,k} D_{hk} \rho_h \left(\frac{\phi_i}{1+\phi_i} \right) \rho_k \left(\frac{\phi_j}{1+\phi_j} \right) \ . \end{aligned} \tag{2.7.41}$$

Now, since condition (2.7.19) implies

$$\sup_h \sum_k |D_{hk}| \leq \frac{1}{1-\alpha} \tag{2.7.42}$$

and we have

$$\rho_h \left(\frac{\phi_i}{1+\phi_i} \right) \leq \rho_h(\phi_i) \leq e^{2J} |J_{i,h}| \tag{2.7.43}$$

we get

$$\begin{aligned} \frac{1}{L}\mathrm{Var}_\pi \left[\sum_{i\in\Lambda} \frac{\phi_i}{1+\phi_i} \right] &\leq e^{4J} \frac{1}{L} \sum_{i,j\in\Lambda} \sum_{h,k\in\Lambda} D_{hk} |J_{i,h}||J_{j,k}| \\ &\leq J^2 e^{4J} \frac{1}{L} \sum_{h,k\in\Lambda} D_{hk} \\ &\leq \frac{1}{1-\alpha} J^2 e^{4J} < \infty \end{aligned} \tag{2.7.44}$$

which completes the proof of Theorem 2.7.1.

2.8 Remarks and open problems on irreversible Kac-Ising dynamics

In the context of one dimensional spin systems with Kac interaction we saw in this chapter how it is possible to define irreversible Markov chains having as stationary measure the Gibbs measure (see Section 2.4) or a measure that, under suitable conditions, tends to the Gibbs measure in the thermodynamic limit (see Section 2.5). Indeed, exploiting the property of magnetization continuity along lattices under periodic boundary conditions, see Section 2.3, we were able to identify the stationary measure of the single spin-flip dynamics with Kac potentials for all values of γ. We have then two different results for parallel dynamics. For nearest neighbors interaction we showed the equivalence of the PCA stationary measure with the gibbsian one by exact computation. In the case of long ranged (Kac) interaction we are able to show such convergence for high temperature via Dobrushin condition.
The interest in this kind of dynamics is twofold: first, it is generally believed (see for example the papers [14] by Dai Pra et al. and [46], [4], [31] by Werner Krauth et al.) that an irreversible sampling of a given measure is faster than a reversible one, and, second, the PCA dynamics are suitable to be implemented on parallel architectures.
However, many questions remain open. Certainly the most interesting one is the possibility to show Theorem 2.7.1 for low temperature, since condition (2.7.1) is fulfilled for high temperature only. It would be also interesting to find explicit estimates for the mixing time both in the reversible and in the irreversible case. In Section 3.3 we show, with this respect, some numerical results about the coalescence times suggesting than the irreversible sampling should be faster that the reversible one.
Beside this, one can think that these irreversible toy models may give some insight in non-equilibrium statistical mechanics. This is in particular the case for the TASEP system, which however is very hard to study once the translational invariance is removed. This thesis should be considered a first attempt in order to find some general results.

Chapter 3

Numerical results

3.1 Markov chains coupling for mixing time estimates

In this chapter we present some numerical results for the two models studied in the theoretical part. In both cases we need to establish a criterion to determine *when* (at what time-step) the dynamics is "close enough" to its steady state, *i. e.* what is its *mixing time*. This section is a quick summary of the *coupling* as a method for estimating such mixing time while a complete reference can be found in [39].
There exist several definitions for the mixing time of a Markov chain, but we hereby proceed to give just the basic principles.

Definition 3.1.1. Consider a Markov chain X^t with state space S and indicate with μ_σ^t the distribution at the time-step t of a dynamics started with the measure μ_σ^0 concentrated on the configuration σ. The mixing time of such dynamics is defined as

$$T := T(\epsilon) = \min_{t>0} \left\{ \|\mu_\sigma^t - \pi\|_{TV} < \epsilon \text{ for all } \sigma \in S \right\} \tag{3.1.1}$$

where π is the stationary measure and ϵ is a small positive parameter, independent on the cardinality of the phase space, often set equal to e^{-1}.

Computing the mixing time of Markov chain can be a non trivial task depending on the dynamics. An effective and widespread method to give an estimate of the value of iterations needed to be "close" to equilibrium is represented by the *coupling*. The coupling is, indeed, a useful and elegant technique in probability theory through which random variables can be compared with each other in order to draw conclusions about their respective distributions. Standard references for coupling methods can be found in Lindvall's and Thorisson's books [43], [1].

Definition 3.1.2. Let X^t and Y^t be two Markov chains on the state space S, then a coupling between X^t and Y^t is another Markov chain $Z^t = (X^t, Y^t)$ with state space $S \times S$ such that

$$P\big(X^{t+1} = \tau \mid Z^t = (\sigma, \sigma')\big) = P\big(X^{t+1} = \tau \mid X^t = \sigma\big) = P_{\sigma\tau} \tag{3.1.2}$$

and

$$P\big(Y^{t+1} = \tau' \mid Z^t = (\sigma, \sigma')\big) = P\big(Y^{t+1} = \tau' \mid Y^t = \sigma'\big) = P_{\sigma'\tau'} \ . \tag{3.1.3}$$

The coupling between X^t and Y^t allows to introduce a dependence between them and to carry out the following general scheme:

1. Define a coupling such that eventually $X^t = Y^t$ with probability 1, *i. e.* $\mathbb{P}_Z(X^t = Y^t) \to 1$ as $t \to \infty$;

2. Bound the total variation distance between π and μ^t_σ in terms of probability $P(X^t \neq Y^t)$ having started X with a measure concentrated in state σ and Y with the stationary measure π;

3. Use this bound to estimate the mixing time $T(\epsilon)$.

Lemma 3.1.1. Let X^t and Y^t be two Markov chains with state space S with initial distributions μ^0 and ν^0, respectively, and $Z^t = (X^t, Y^t)$ be a coupling on them. Then

$$\|\mu^t - \nu^t\|_{TV} \leq P\big(X^t \neq Y^t\big) \ . \tag{3.1.4}$$

Proof. Given any $A \subset S$, we have

$$\begin{aligned} \mu^t(A) - \nu^t(A) &= P(X^t \in A) - P(Y^t \in A) \\ &= P(X^t \in A, Y^t \notin A) - P(Y^t \in A, X^t \notin A) \\ &\leq P(X^t \in A, Y^t \notin A) \\ &\leq P(X^t \neq Y^t) \ . \end{aligned} \tag{3.1.5}$$

□

Applying Lemma 3.1.1 with the initial distribution μ^0 concentrated on a single state $\sigma \in S$, and with ν^0 being the stationary distribution π gives the estimate

$$\|\mu^t_\sigma - \pi\|_{TV} \leq P\big(X^t \neq Y^t\big) \ . \tag{3.1.6}$$

Therefore, for a time-step T such that

$$P\big(X^T \neq Y^T \mid X^0 = \sigma, Y^0 \text{ distributed according to } \pi\big) \leq \epsilon \tag{3.1.7}$$

we have $T(\epsilon) \leq T$, which is the estimate of the mixing time of the Markov chain.

From a numerical point of view this technique is a powerful tool to understand how many iterations are enough to be confident that a simulation of a dynamics has reached its steady state. Constructing two or more processes on the same probability space and updating them with the same variables, *i. e.* the extracted site and the random number to compare with the transition probability, we are sure that after the *coalescence* the Markov chain will remain equal during all the future evolution independently from the starting state.
Setting the starting configurations of the Markov chains "as far as possible" one from the other, *e. g.* in discrete spin systems the $+1$ and the -1 states, the time needed for them to be equal is a good indication of the mixing time. Furthermore, if the update rule preserves the partial order between the configurations, starting the coupling from the "top" state (all $+1$) and the "bottom" state (all -1) ensures that *all* the chains starting in any intermediate states have to join as well. This is the so called *sandwiching* technique, see [26], and allows to compute an upper bound for the mixing time without running the coupling for all the intermediate configurations.

3.2 PCA-TASEP

The classical TASEP model imposes that exactly one particle is chosen uniformly at each iteration and moved forward if not blocked by another particle. In big volume instances of the problem this means that the whole dynamics results to be very slow.
Adopting the parallel PCA dynamics for the classic discrete-time TASEP increases enormously its capability to be implemented on the calculator and to be studied numerically. We will show how the parallelization doesn't change the model qualitatively but only quantitatively, making it get faster to the stationary state than the classical version.
We present a series of numerical results obtained in a half-filled PCA-TASEP system, with blockage probability $\varepsilon \in [0, 1]$ located on the last site $i = 2L$, on a ring lattice of 1000 sites and 500 particles. In particular we will compute experimentally the current $J(p, \varepsilon)$ and the density $\rho(x, p, \varepsilon)$ around the site x, as functions of both the probability $p = \frac{w}{1+w}$ and the blockage's intensity ε. The current is computed according to (1.3.2), while the density in $x \in \{1, 2, \ldots, {}^{2L}/_{10}\}$ is defined as follows

$$\rho(x, p, \varepsilon) = \frac{1}{10} \left[\sum_{i=10x}^{10x+9} \sigma_i \right] . \tag{3.2.1}$$

To guarantee the achievement of the stationary state we need to run the simulation for the *mixing time* of the PCA-TASEP, hereby simply referred as T. Unfortunately we are not aware of rigorous estimate of the mixing time for the serial dynamics nor the parallel one. In the case of the symmetric exclusion process on the circle, in [48] Morris proved that $T = L^2 \log L$, and this corresponds in our case to the choice $p = {}^1/_{2L}$. Therefore, we can imagine that a PCA-TASEP dynamics with jump probability p will have a mixing time approximately

$$T \approx 2 \, \frac{L}{p} \, log(L) \, . \tag{3.2.2}$$

To test such estimate we implemented the procedure described in Section 3.1 and performed a numerical simulation. As widely explained, the PCA-TASEP is a parallel Markov chain of the class of PCA, *i. e.* its update rule is factorized on the single sites i. This feature makes the dynamics particularly well suited to be implemented on Graphical Processors Units (GPUs) without time-consuming inter-thread dependencies. In other words, they are eligible for large scale simulations on relatively cheap computing architectures like graphics cards.
Figure 3.1 is the result of a simulation executed within the CUDA[1] framework of 10^5 couplings, referred as *rings* in the x-axis of the figure, of the

[1] https://developer.nvidia.com/cuda-zone

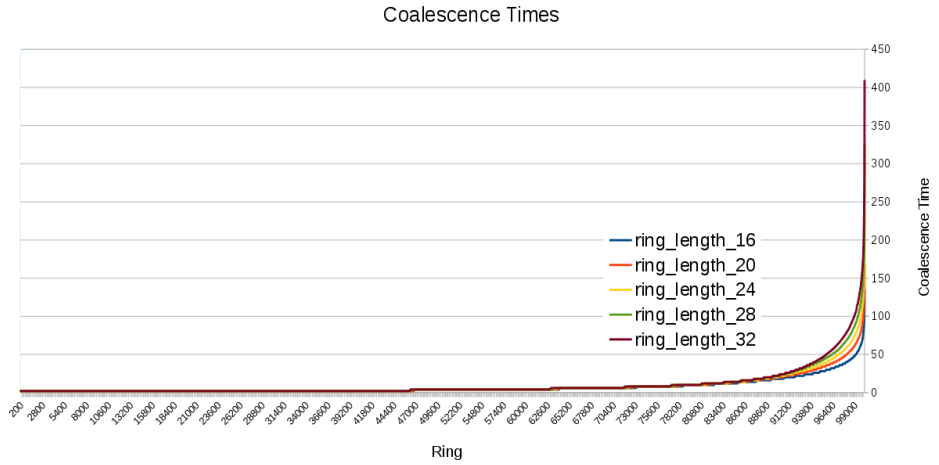

Figure 3.1: Coalescence times for the PCA-TASEP with periodic bounday conditions (the lattice is a ring) of 10^5 rings of volume $16, 20, 24$ and 28.

PCA-TASEP parallel dynamics for different volume sizes and returns their coalescence times, plotted on the y-axis. Exploiting the parallel capabilities of the GPU both within the parallel update rule of each coupling and also executing 1000 couplings at once, we were able to obtain a statistic sample of 10^5 coalescence times for volume sizes $16, 20, 24, 28, 32$ in just 10^2 runs of the simulator. Obtaining coalescence times for bigger volumes begins to be unfeasible and its beyond the purposes of the simulation. The final version of the code is given in Appendix B.1.
The fact that in no one of the 10^5 instances of the coupling the coalescence time exceeded the estimate (3.2.2) is an indication that running the simulation for, at least, that number of iterations implies the attainment of a stationary state. Hence, in the following simulations we run the dynamics for a time greater than $^{2L}/_{p}\ \log(L)$.

In our numerical experiments we are particularly interested on two facts:

1. We know from [13] that for the standard TASEP the current remains very close to the limit value without blockage, up to a certain value ε_c of the blockage intensity. We also know from Theorem 1.4.1, that for the explicitly solvable blocked system, in the case $p = 1$ there is no critical blockage probability, in the sense that the current has a decrease that is proportional to ε near the value $\varepsilon = 0$.

   We want to check numerically if the indication of such $\varepsilon_c \neq 0$ is a particular feature of the single spin flip dynamics or if it survives in the PCA procedure too. As it will be clear in the following figures, the second scenario seems to be true from a numerical point of view.

2. We want to see if the density before the blockage is an increasing function of the distance from the blockage when the current decreases, or if the presence of the blockage implies simply a *queuing* of particles close to it.

3.2.1 Current

The measure of the current J is carried out, according to formula (1.3.2, counting the average number of particles free to move during all the iterations and weighting such value with the total volume of the system $2L$.

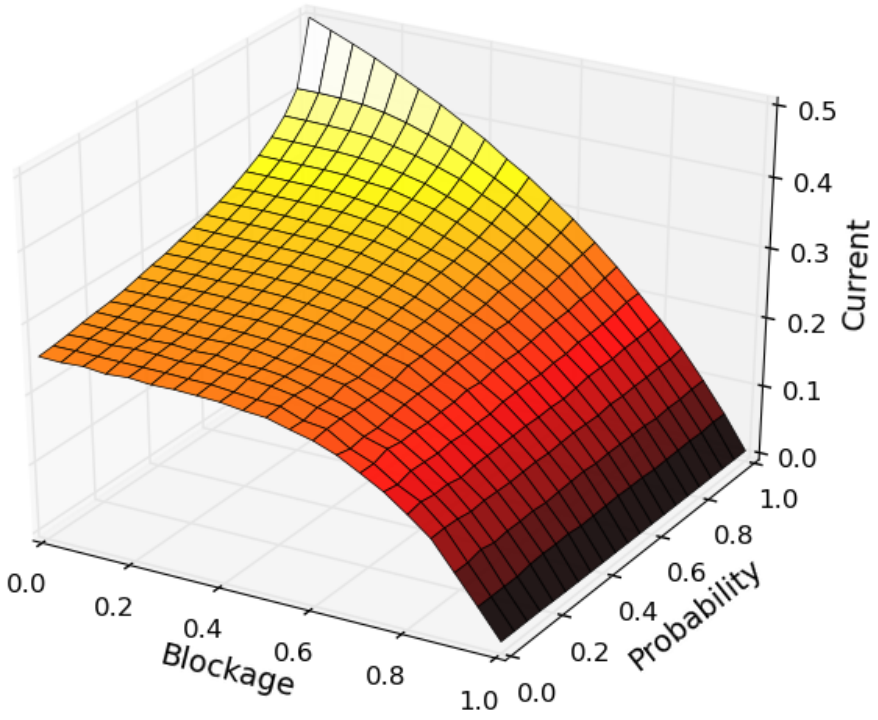

Figure 3.2: Current in PCA-TASEP as function of the probability $p = {}^{w}/_{(1+w)}$ and the blockage intensity ε.

Figure 3.2 shows the surface obtained interpolating 441 measures of $J(p, \varepsilon)$ for every $p \in [\frac{1}{2L}, ..., 1]$ and $\varepsilon \in [0, ..., 1]$, both with increments of ${}^{25}/_{L} = 0.05$. As we see, the Current-Blockage plane of the 3D graph fits very well the relations shown in Proposition 1.3.1 and Theorem 1.4.1, both in the $p = 1$ and $p = \frac{1}{L}$ cases.
Figure 3.3 represents the behavior of the current $J(p, \varepsilon)$ for several values of p plotting the side projection of the 3D graph from Figure 3.2. It clearly

appears that except in the case $p = 1$, where the current decrease with a non-zero slope for all $\varepsilon > 0$, the decrease of $J(p, \varepsilon)$ starts only after a certain value of the blockage.

In this sense, the critical behavior of the standard TASEP, corresponding in our model to the regime $p = \frac{1}{L}$, is conserved for all the probabilities except $p = 1$.

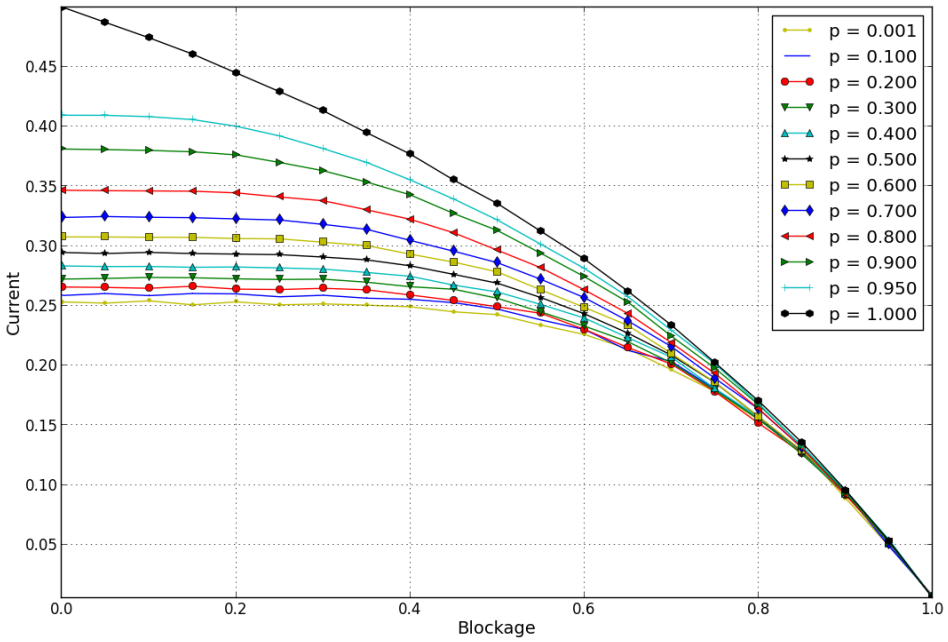

Figure 3.3: Profile curves of the PCA-TASEP current for different values of the probability p, from $p = 1$ (up) to $p = \frac{1}{L}$ (down).

Figure 3.4 shows the threshold values of ε for which the current deviates more than the 1% from its initial value in the absence of blockage. This gives an indication of the shape of the region in which the current remains nearly constant from a numerical point of view, having however $\varepsilon > 0$. Note that the dots have a monotone behavior as to higher mobility rates correspond a system more sensible to the blocking effect in the end of the volume.

Again, it seems from the simulations that for every value of p ,except $p = 1$ for which the slope of the current is clearly negative already at $\varepsilon = 0$, it exists a critical blockage intensity ε_c. However the recent developments in [3], [2] proves that such ε_c is indeed 0, leaving open the conjecture of the non-analyticity of $J(p, \varepsilon)$.

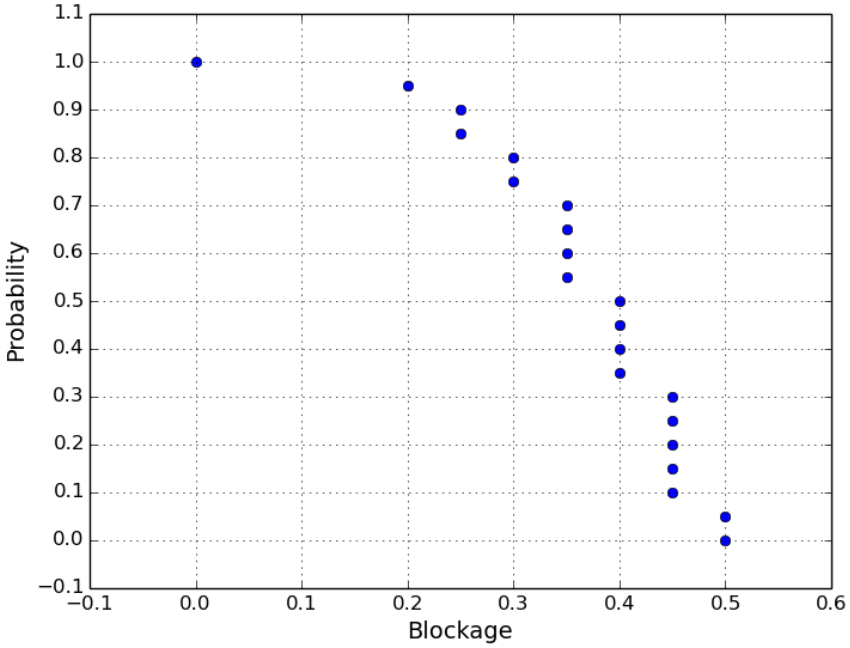

Figure 3.4: Threshold values of ε for a 1% deviation from value of the current without blockage.

3.2.2 Density

The second feature we focused on is the distribution of the particles in the whole volume during the evolution of the system. The density diagrams we are going to show describe the density of segments of the configuration, assigning a darker color according to the density. We suppose that a good choice for the coarse-graining of the volume is to have segments of length 10 in order to have 100 samples to look at and still a representative basis to measure the concentration of particles.
The diagrams in Figure 3.5, are an instantaneous plot of the configuration σ at the *mixing time* defined in (3.2.2) for each probability p as defined above the plot. Each diagram is composed of 6 tiny rows showing the particle density for $\varepsilon \in \{0, 0.2, 0.4, 0.6, 0.8, 1\}$. As we expected the last row of every diagram is split in half *white-empty* and half *black-full* dots, due the total congestion of the ring when $\varepsilon = 1$.
Figure 3.6 plots the average behavior from 100 density diagrams computed every 100 iterations after the system reached the steady state. Exactly like the previous graph, the first row correspond to the complete absence of blockage and its uniform gray color fairly reflects this situation showing a uniform distribution of the particles.

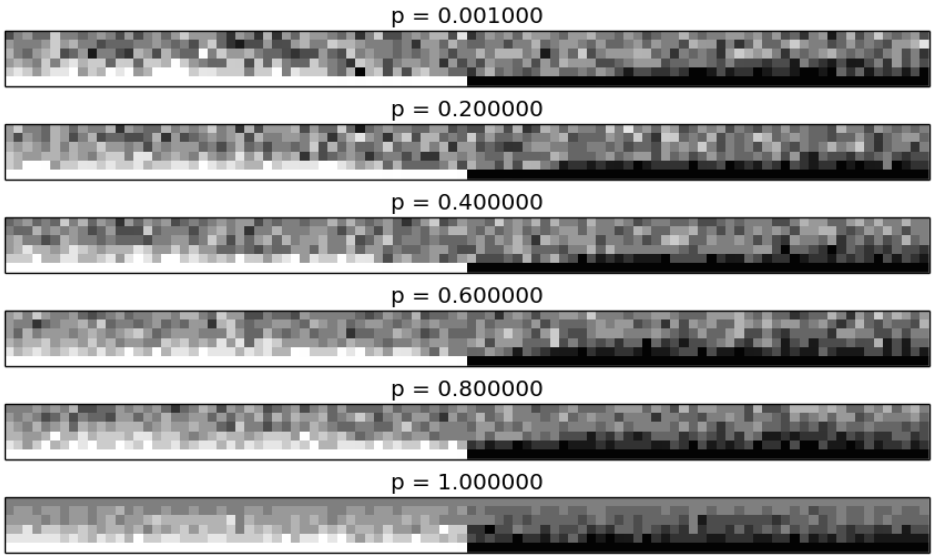

Figure 3.5: Average site occupation (density) for the PCA-TASEP at different values of blockage ε.

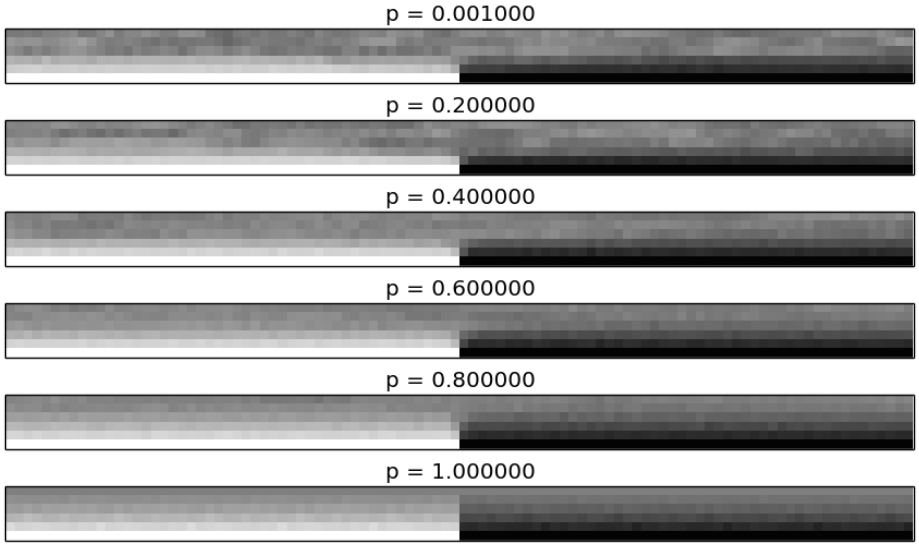

Figure 3.6: Mean density for 100 steps of 100 iterations each, after the *Mixing Time*.

All the evidence seems to indicate the possibility that, although the current decreases for all ε, the system exhibits for $p < 1$ a nearly-constant density up to a certain value of ε, while after this value the density appears to be smaller in the first L sites than in the second L. Such a difference in the density of the two halves of the ring is precisely what has emerged in Section 1.4 for the case $p = 1$ with an arbitrary blockage-intensity $\varepsilon > 0$, where the particle-hole symmetry plays a key role. Again, a complete understanding of this phenomenon should be based on the knowledge of the stationary measure in presence of a blockage.

3.3 Kac-Ising

For what concerns the Kac-Ising model we focused on a numerical comparison of the speed of convergence to equilibrium between the reversible and irreversible dynamics. Differently from the previous model, in this case we deal with single spin-flip dynamics because we are interested on testing the general belief that an irreversible sampling of a given measure is faster than a reversible one. We wrote a script in Ruby language for the computation of the coalescence times and, exploiting the multi-processors architecture and the parallel nature of the statistical sampling, we managed to run 64 couplings in parallel, one on each available CPU.

In order to apply the *sandwiching* technique described in Section 2.4 we need a coupling that preserves the partial order during the evolution of the configurations.

Proposition 3.3.1. Call U_i^t a family of i.i.d. random variables uniformly distributed in $(0,1)$ and define the update scheme of the site i at the time-step t for the two configurations σ, τ as follows:

- flip σ_i if $U_i^t < e^{-2\beta(m_i(\sigma)\sigma_i + a)}$;
- flip τ_i if $U_i^t < e^{-2\beta(m_i(\tau)\tau_i + a)}$ and $\sigma_i = \tau_i$;
- flip τ_i if $U_i^t > 1 - e^{-2\beta(m_i(\tau)\tau_i + a)}$ and $\sigma_i = -\tau_i$;
- in any other case we leave σ_i, τ_i unaltered.

Then, initializing the Markov chains with the configurations $\sigma^0 : \sigma_i^0 = -1,\ \tau^0 : \tau_i^0 = +1\ \forall i$ and setting $a > 1 + \frac{\log(2)}{2\beta}$, the coupling defined above preserves the partial order between σ, τ.

Proof. We want to show that $\sigma^t \preceq \tau^t$, *i. e.* $\sigma_j^t \leq \tau_j^t\ \forall j$, at all the time-steps t. Clearly that's true at $t = 0$, therefore we have to prove that all these events are impossible:

- flipping σ_i from -1 to $+1$ keeping $\tau_i = -1$ unflipped;
- flipping τ_i from $+1$ to -1 keeping $\sigma_i = +1$ unflipped;
- flipping σ_i from -1 to $+1$ while flipping τ_i from $+1$ to -1.

Since $\sigma^t \preceq \tau^t$ implies $m_i(\sigma) \leq m_i(\tau)$, the first and second case are trivial because the event $\left(\sigma_i^t = +1 | \sigma_i^{t-1} = -1\right)$ happens when

$$U_i^t < e^{-2\beta(a - m_i(\sigma))} < e^{-2\beta(a - m_i(\tau))} \tag{3.3.1}$$

which implies $\left(\tau_i^t = +1 | \tau_i^{t-1} = -1\right)$ and, similarly, $\left(\tau_i^t = -1 | \tau_i^{t-1} = +1\right)$ happens when

$$U_i^t < e^{-2\beta(a + m_i(\tau))} < e^{-2\beta(a + m_i(\sigma))} \tag{3.3.2}$$

which implies $\left(\sigma_i^t = -1 | \sigma_i^{t-1} = +1\right)$.
The event $\left(\sigma_i^t = +1 | \sigma_i^{t-1} = -1\right) \cup \left(\tau_i^t = -1 | \tau_i^{t-1} = +1\right)$ could only happen when

$$U_i^t < e^{-2\beta\left(a - m_i(\sigma)\right)} \ \vee \ U_i^t > 1 - e^{-2\beta\left(a + m_i(\tau)\right)}, \tag{3.3.3}$$

but that's not possible because, having set $a > 1 + \frac{\log(2)}{2\beta}$, we have

$$e^{-2\beta\left(m_i(\sigma)\sigma_i + a\right)} + e^{-2\beta\left(m_i(\tau)\tau_i + a\right)} < 1 \tag{3.3.4}$$

therefore there's no intersection for U_i^t to be, see Figure 3.7 below.

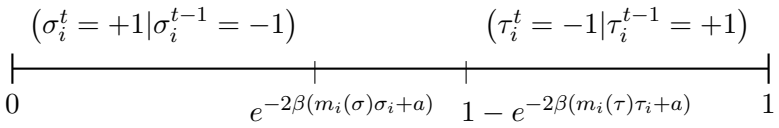

Figure 3.7: Probabilities of the event of flipping σ_i from -1 to $+1$ while flipping τ_i from $+1$ to -1.

□

Figures 3.8, 3.9, 3.10 show the results of 20000 couplings at different β and γ for two versions of the same dynamics: one that updates each site according to its *symmetric* local field, *i. e.* the average magnetization of the sites at distance γ^{-1} in both left and right directions, and the other for its *asymmetric* local field, *i. e.* only on the right. The results agrees with the conjecture that irreversible dynamics *mix* faster than the reversible ones and also indicates that such speedup increases with β, *i. e.* at low temperature, and also with γ^{-1}. This feature suggests that the irreversible sampling can be a valid candidate to replace the classical reversible ones having better performance in the usually most interesting regions of parameters, low temperature and long interaction.

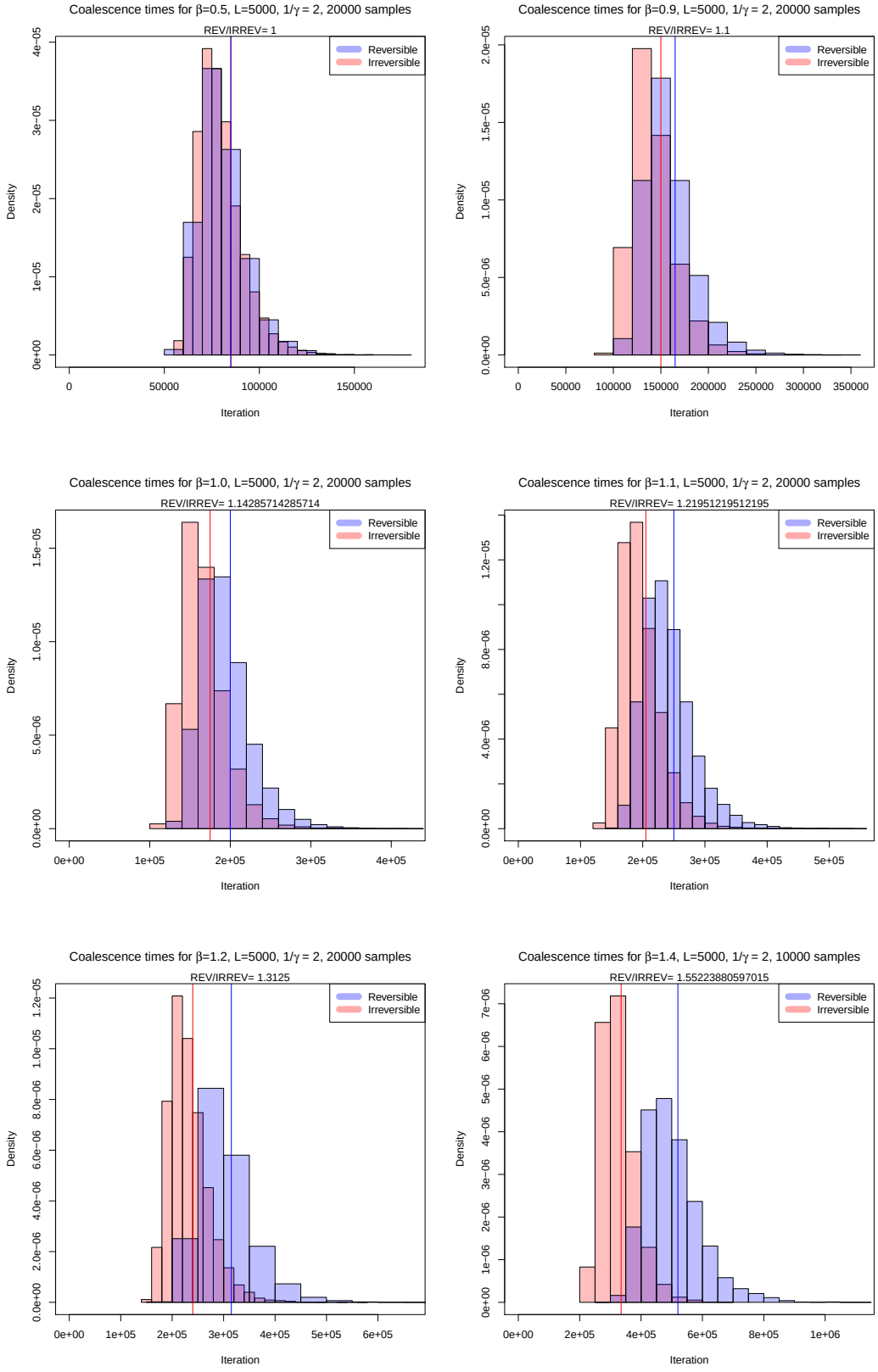

Figure 3.8: Coalescence times for reversible and irreversible single spin-flip Kac-Ising dynamics for $\beta = 0.5, 0.9, 1.0, 1.1, 1.2, 1.4$ and $\gamma^{-1} = 2$.

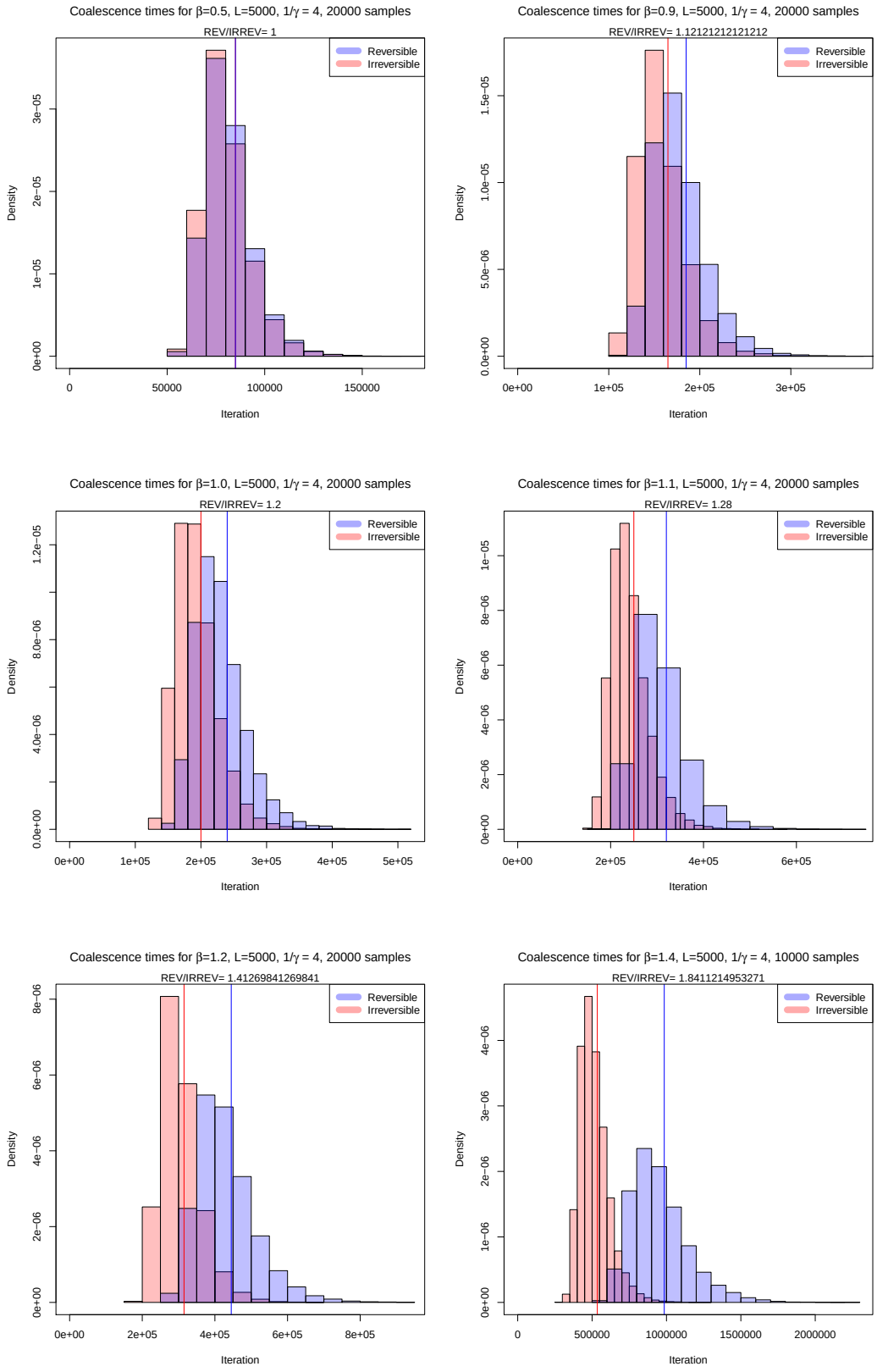

Figure 3.9: Coalescence times for reversible and irreversible single spin-flip Kac-Ising dynamics for $\beta = 0.5, 0.9, 1.0, 1.1, 1.2, 1.4$ and $\gamma^{-1} = 4$.

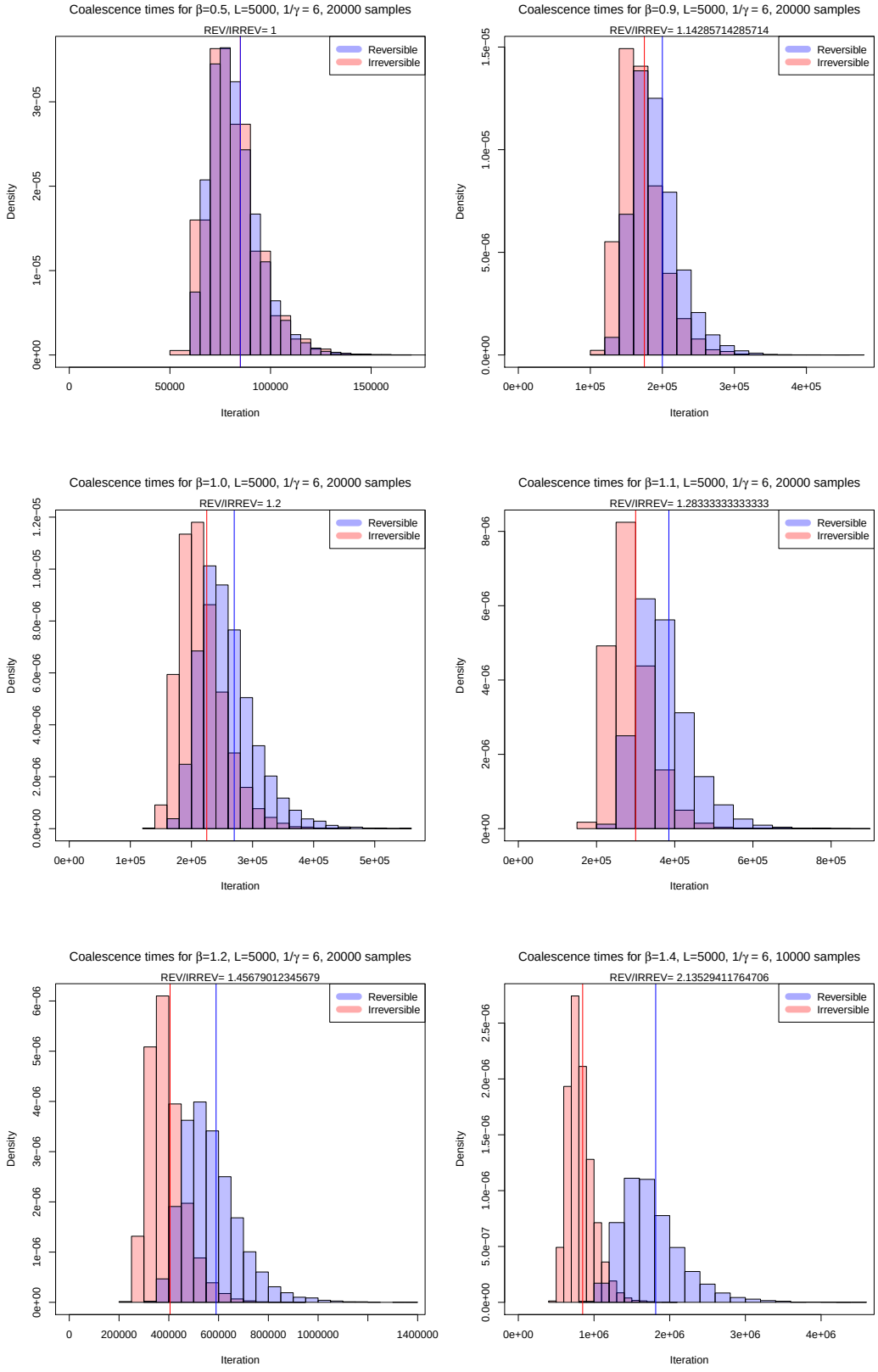

Figure 3.10: Coalescence times for reversible and irreversible single spin-flip Kac-Ising dynamics for $\beta = 0.5, 0.9, 1.0, 1.1, 1.2, 1.4$ and $\gamma^{-1} = 6$.

Appendices

Appendix A

Föllmer Theorem

In this appendix we show and prove the covariance estimate presented by Föllmer in [21] and used in Theorem (2.7.2). The proof builds on a variant of Dobrushin's comparison theorem, see [18], we present in Section A.1 and uses an estimate of the Kantorovich distance we show in A.2.

A.1 Dobrushin Uniqueness Theorem

For two probability measures μ and ν on a countable product space E suppose the following:

- μ is a probability measure on a product space $E = S^I$ and we know for all points $k \in I$ the conditional distributions $\mu_k(dx_k|x)$;
- ν is another measure which does not have to be Gibbsian but its conditional probabilities $\nu_k(\cdot|x)$ must exist;
- C is the so called *Dobrushin interaction matrix* with elements

$$C_{ik} = \sup\left\{\tfrac{1}{2}\|\mu_k(\cdot|x) - \mu_k(\cdot|y)\|_1 : x = y \text{ off } \{i\}\right\} \tag{A.1.1}$$

  and we suppose the following condition holds

$$\alpha = \sup_k \sum_i C_{ik} < 1 \ ; \tag{A.1.2}$$

- D is the matrix with elements $D_{ik} = \sum_{n=0}^{\infty} C^n$;
- the so called *oscillation* of f in the point i is defined as

$$\delta_i(f) = \sup\Big\{|f(x) - f(y)| : x = y \text{ off } \{i\}\Big\} \ ; \tag{A.1.3}$$

- and b is the vector such that

$$b_k = \tfrac{1}{2} \int \|\mu_k(\cdot|x) - \nu_k(\cdot|x)\|_1 \; \nu(dx) \; . \tag{A.1.4}$$

Theorem A.1.1. Under condition (A.1.2) we have

$$\left| \int f d\mu - \int f d\nu \right| \leq \sum_{i \in I} (bD)_i \, \delta_i(f) \qquad \big(f \in C(E)\big) \; . \tag{A.1.5}$$

In the following proof we will use the notation $\mu_k(f|x) = \int f \mu_k(dx_k|x)$, which in probability theory is commonly written as the conditional expectation $\mathbb{E}_\mu \left[f | \Sigma_{\neq k} \right](x)$ of the measure μ with respect to the σ-algebra, generated by the random variables that are different from x_k computed on the point x of the sample space E. We will also need the following lemmata.

Lemma A.1.1. If μ_1 and μ_2 are two probability measures on the phase space Ω, defining $c = c(f) = \frac{1}{2} (\sup f + \inf f)$ for every $f \in C(E)$ we have that

$$\begin{aligned} |\mu_1(f) - \mu_2(f)| &= |(\mu_1 - \mu_2)(f - c)| \\ &\leq \|\mu_1 - \mu_2\|_1 \; \sup |f - c| \\ &= \|\mu_1 - \mu_2\|_1 \; \tfrac{1}{2} \, |\sup f - \inf f| \; . \end{aligned} \tag{A.1.6}$$

A vector $a = (a_i)_{i \in I}$ will be called an *estimate* for two probability measures μ and ν if

$$\left| \int f d\mu - \int f d\nu \right| \leq \sum_{i \in I} a_i \delta_i(f) \qquad \forall f \in C(E) \; . \tag{A.1.7}$$

Lemma A.1.2. If a is an estimate for μ and ν, then the vector $(aC + b)$ is also an estimate for μ and ν.

Proof. Let J be a set of points in I and define a^J by

$$a_i^J = \begin{cases} \min \big(a_i, (aC + b)_i\big) & (i \in J) \\ a_i & (i \notin J) \; . \end{cases} \tag{A.1.8}$$

Remark A.1.1. Note that $a^\emptyset = a$ since $i \notin J = \emptyset \implies a_i^\emptyset = a_i$ which we supposed is an estimate.

Clearly if we prove that a^J is an estimate for μ and ν for every $J \subset I$ we showed that $(aC + b)$ is also an estimate for μ and ν. We proceed by induction on the cardinality of J:

1. for $J = \emptyset$, as said in Remark A.1.1, a^J is an estimate for μ and ν;
2. we have to show that if a^J is an estimate for μ and ν (for a given $J \neq \emptyset$) then also a^K is an estimate for μ and ν, where $K = J \cup \{k\}$.

For $f \in C(E)$ we have, by definition,

$$\begin{aligned}\left| \int f d\mu - \int f d\nu \right| = & \left| \int \mu_k(f|x)\mu(dx) \right. \\ & \left. - \int \nu_k(f|x)\nu(dx) \right| \ .\end{aligned} \tag{A.1.9}$$

Adding inside the modulus on the r.h.s of (A.1.9)

$$0 = \int \mu_k(f|x)\nu(dx) - \int \mu_k(f|x)\nu(dx) \ , \tag{A.1.10}$$

using the triangular inequality and grouping conveniently the terms, we obtain

$$\begin{aligned}\left| \int f d\mu - \int f d\nu \right| \leq & \left| \int \mu_k(f|x)(\mu - \nu)(dx) \right| \\ & + \int |\mu_k(f|x) - \nu_k(f|x)|\nu(dx) \ .\end{aligned} \tag{A.1.11}$$

For simplicity from now on we will refer to the terms of (A.1.11) as

$$\mathrm{I} = \left| \int \mu_k(f|x)(\mu - \nu)(dx) \right| \tag{A.1.12}$$

and

$$\mathrm{II} = \int |\mu_k(f|x) - \nu_k(f|x)|\nu(dx) \ . \tag{A.1.13}$$

To find an estimate for (A.1.12) we use the definition of estimate for μ and ν given in (A.1.7) to write

$$\left| \int \mu_k(f|x)(\mu - \nu)(dx) \right| \leq \sum_i a_i \delta_i\big(\mu_k(f|\cdot)\big) \tag{A.1.14}$$

where, provided that $i \neq k$, we have that

$$\delta_i\big(\mu_k(f|\cdot)\big) = \sup \left| \mu_k(f|x) - \mu_k(f|y) \right| : x = y \text{ off } \{i\} \ . \tag{A.1.15}$$

Suppose, now, that $\{s, t\}$ are two configurations, *i. e.* two points on E, which coincide everywhere except the point $\{i\}$: $\big\{s, t : s = t \text{ off } \{i\}\big\}$.
We can compute (A.1.15) as done by Gross in [25] as follows

$$\mu_k(f|\cdot) = \int f(x \circ_{\mathrm{k}} s)\mu_k(dx|s) \tag{A.1.16}$$

where $(x \circ_{\mathrm{k}} s)$ denotes the configuration taking the value x_k in the point k and which is s everywhere else.
The argument of the r.h.s. of equation (A.1.15) can then be written as

$$\Big|\mu_k(f|s) - \mu_k(f|t)\Big| = \left|\int f(x \circ_{\mathrm{k}} s)\mu_k(dx|s) - \int f(x \circ_{\mathrm{k}} t)\mu_k(dx|t)\right| \quad \text{(A.1.17)}$$

for any point $i \neq k$.
Adding inside the modulus of (A.1.17)

$$0 = \int f(x \circ_{\mathrm{k}} t)\mu_k(dx|s) - \int f(x \circ_{\mathrm{k}} t)\mu_k(dx|s) \ , \quad \text{(A.1.18)}$$

using the triangular inequality and grouping conveniently the terms we obtain

$$\begin{aligned} |\mu_k(f|s) - \mu_k(f|t)| \leq & \left|\int \Big(f(x \circ_{\mathrm{k}} s) - f(x \circ_{\mathrm{k}} t)\Big)\mu_k(dx|s)\right| \\ & + \left|\int f(x \circ_{\mathrm{k}} t)\Big(\mu_k(dx|s) - \mu_k(dx|t)\Big)\right| \ . \end{aligned} \quad \text{(A.1.19)}$$

On the one hand, for $i \neq k$ we have that

$$\begin{aligned} & \left|\int \Big(f(x \circ_{\mathrm{k}} s) - f(x \circ_{\mathrm{k}} t)\Big)\mu_k(dx|s)\right| \\ & \qquad \leq \sup\Big\{|f(s) - f(t)| : s = t \text{ off } \{i\}\Big\} \\ & \qquad = \delta_i(f) \ . \end{aligned} \quad \text{(A.1.20)}$$

On the other hand, using Lemma A.1.1, we have

$$\begin{aligned} & \left|\int f(x \circ_{\mathrm{k}} t)\Big(\mu_k(dx|s) - \mu_k(dx|t)\Big)\right| \\ & \qquad \leq \sup_{s,t}\Big\{\|\mu_k(\cdot|s) - \nu_k(\cdot|t)\|_1 \ \tfrac{1}{2}|\sup(f) - \inf(f)|\Big\} \\ & \qquad = C_{ik}\delta_k(f) \end{aligned} \quad \text{(A.1.21)}$$

since in our case

$$\begin{aligned} \Big|\sup(f) - \inf(f)\Big| &= \Big|\sup_x\big(f(x \circ_{\mathrm{k}} t)\big) - \inf_x\big(f(x \circ_{\mathrm{k}} t)\big)\Big| \\ &= \sup\Big\{|f(s') - f(t)| : s' = t \text{ off } \{k\}\Big\} \\ &= \delta_k(f) \ . \end{aligned} \quad \text{(A.1.22)}$$

Therefore, we obtain

$$\Big|\mu_k(f|s) - \mu_k(f|t)\Big| \leq \delta_i(f) + C_{ik}\delta_k(f) \quad \text{with } s = t \text{ off } \{i\} \ . \quad \text{(A.1.23)}$$

Recalling definition (A.1.3) we have

$$\delta_i\big(\mu_k(f|\cdot)\big) = \sup\left\{\Big|\mu_k(f|s) - \mu_k(f|t)\Big| : s = t \text{ off } \{i\}\right\} \tag{A.1.24}$$

and, immediately, it follows that

$$\delta_i\big(\mu_k(f|\cdot)\big) \leq \delta_i(f) + C_{ik}\delta_k(f)\ . \tag{A.1.25}$$

Moreover, since the integral $\mu_k(f|s) = \int f d\mu_k(\cdot|s)$ is independent of s_k, if $i = k$ the difference in the l.h.s of (A.1.23) is zero, *i. e.*

$$\Big|\mu_k(f|s) - \mu_k(f|t)\Big| = 0 \quad \text{with } s = t \text{ off } \{i\} \text{ or } \{k\} \tag{A.1.26}$$

thus

$$\delta_i\big(\mu_k(f|\cdot)\big) \leq \begin{cases} \delta_i(f) + C_{ik}\delta_k(f) & \text{if } i \neq k, \\ 0 & \text{otherwise.} \end{cases} \tag{A.1.27}$$

Let's now find an estimate for (A.1.13). Using again Lemma A.1.1 we can write

$$\begin{aligned} &\int \Big|\mu_k(f|x) - \nu_k(f|x)\Big|\nu(dx) \\ &\leq \int \Big|\|\mu_k(\cdot|x) - \nu_k(\cdot|x)\|_1\ \tfrac{1}{2}\big|\sup f - \inf f\big|\Big|\nu(dx) \\ &\leq \sup\Big\{\big|f(x) - f(y)\big| : x = y \text{ off } \{k\}\Big\}\ \tfrac{1}{2}\int \|\mu_k(\cdot|x) - \nu_k(\cdot|x)\|_1\nu(dx) \\ &= \delta_k(f)b_k \end{aligned} \tag{A.1.28}$$

where we have used (A.1.22).
At this point, recalling equation (A.1.27), we have

$$\begin{aligned} \left|\int f d\mu - \int f d\nu\ \right| &\leq \mathrm{II} + \mathrm{I} \\ &= b_k\delta_k(f) + \sum_i a_i\left[\delta_i(f) + C_{ik}\delta_k(f)\right] \\ &= (aC + b)_k\,\delta_k(f) + \sum_{i\neq k} a_i\delta_i(f)\ . \end{aligned} \tag{A.1.29}$$

By induction hypothesis we have that

$$\left|\int f d\mu - \int f d\nu\ \right| \leq a_k^J\delta_k(f) + \sum_{i\neq k} a_i^J\delta_i(f) \tag{A.1.30}$$

so the best of the two estimates is

$$\begin{aligned}\left|\int f d\mu - \int f d\nu \right| &\leq \min\left(a_k^J, \left(a^J C + b\right)_k\right) \delta_k(f) + \sum_{i\neq k} a_i^J \delta_i(f) \\ &= a_k^K \delta_k(f) + \sum_{i\neq k} a_i^K \delta_i(f) \\ &= \sum_i a_i^K \delta_i(f) \ .\end{aligned} \tag{A.1.31}$$

Thus, if a^J is an estimate for μ and ν also a^K is an estimate for μ and ν, where $K = J \cup \{k\}$, which completes the proof of Lemma A.1.2. □

Proof of Theorem A.1.1. Applying Lemma A.1.2 recursively we obtain that every vector a^n such that

$$\begin{aligned} a^0 &= a \\ a^1 &= (a_0 C + b) = (aC + b) \\ a^2 &= (a_1 C + b) = \big((aC + b)C + b\big) \\ &\cdots \\ a^n &= aC^n + b \sum_{m=0}^{n} C^m \end{aligned} \tag{A.1.32}$$

is an estimate and since, in the limit $n \to \infty$ and under condition (A.1.2), we have

$$aC^n \to 0 \quad \text{and} \quad b \sum_{m=0}^{n} C^m \to bD \ . \tag{A.1.33}$$

Therefore

$$|\mathrm{Cov}_\mu(f,g)| = \left|\int f d\mu - \int f d\nu \right| \leq \sum_i (bD)_i \delta_i(f) \qquad \big(f \in C(E)\big)$$

which completes the proof of Theorem A.1.1. □

Remark A.1.2. If μ and ν have same the conditional probabilities then $b = 0$ and that implies $\mu = \nu$, and this is Dobrushin's uniqueness theorem.

A.2 Covariance estimate via Kantorovich distance

To complete the proof of Theorem 2.7.2 it remains to show that, using the appropriate metrics, we can estimate the variance between two measures μ and ν as

$$\left|\mathrm{Cov}_\mu(f,g)\right| \leq \tfrac{1}{4}\sum_{i,k}\rho_i(f)D_{ik}\rho_k(g)\ .$$

Define the Rubinstein-Kantorovich distance as follows

$$R(\mu,\nu) = \sup_f \frac{\left|\int f d\mu - \int f d\nu\right|}{\delta(f)} \tag{A.2.1}$$

where, as before,

$$\delta(f) = \sup_{s\neq t}\frac{|f(s)-f(t)|}{r(s,t)} \tag{A.2.2}$$

is the so called *oscillation* of f and $r(s,t)$ is a metric

Remark A.2.1. If such metric is *discrete*, *i. e.* $r(s,t) = \mathbb{1}_{\{s\neq t\}}$, clearly

$$\delta(f) = \sup_{s\neq t}|f(s)-f(t)| = \sup(f) - \inf(f) \tag{A.2.3}$$

and, by Lemma A.1.1,

$$R(\mu,\nu) = \tfrac{1}{2}\|\mu-\nu\|_1\ . \tag{A.2.4}$$

Recalling the definition of covariance for two functions $f, g \in L(\mu)^2$, if two measures μ and ν are such that $d\nu = gd\mu$ we have

$$\begin{aligned}\mathrm{Cov}_\mu(f,g) :&= \int fg\ d\mu - \int f\ d\mu \int g\ d\mu \\ &= \int f\ d\nu - \int f\ d\mu \int d\nu \\ &= \int f\ d\nu - \int f\ d\mu\ .\end{aligned} \tag{A.2.5}$$

We can then write, by Cauchy-Schwarz inequality,

$$\left|\int f\ d\nu - \int f\ d\mu\right| = \left|\mathrm{Cov}_\mu(f,g)\right| \leq \mathrm{Var}_\mu(f)^{\frac{1}{2}}\mathrm{Var}_\mu(g)^{\frac{1}{2}}\ . \tag{A.2.6}$$

Lemma A.2.1. The variance of a function g with respect to a measure μ can be written as

$$\mathrm{Var}_\mu(g) = \inf_\alpha \int (g-\alpha)^2\ d\mu\ . \tag{A.2.7}$$

Proof. Let's find the value $\bar{\alpha}$ that minimizes

$$\int (g-\alpha)^2 \, d\mu = \int g^2 \, d\mu + \int \alpha^2 \, d\mu - 2\int g\alpha \, d\mu \; . \tag{A.2.8}$$

Deriving the expression we obtain

$$\frac{d}{d\alpha}\int (g-\alpha)^2 \, d\mu = 2\int \alpha \, d\mu - 2\int g \, d\mu \tag{A.2.9}$$

and substituting α with $\int g \, d\mu$ we have

$$\begin{aligned}
\inf_{\alpha} \int (g-\alpha)^2 \, d\mu &= \inf_{\alpha} \int \left(g^2 + \alpha^2 - 2g\alpha\right) \, d\mu \\
&= \int g^2 \, d\mu + \int \left(\int g \, d\mu\right)^2 \, d\mu - 2\int g \left(\int g \, d\mu\right) \, d\mu \\
&= \int g^2 \, d\mu + \left(\int g \, d\mu\right)^2 - 2\left(\int g \, d\mu\right)^2 \\
&= \int g^2 \, d\mu - \left(\int g \, d\mu\right)^2 = \mathrm{Var}_{\mu}(g) \; .
\end{aligned} \tag{A.2.10}$$

□

Since $g(x) \leq \sup_x \{g(x)\}$ we clearly have that

$$g(x) - \tfrac{1}{2}(\sup g + \inf g) \leq \tfrac{1}{2}(\sup g - \inf g) \leq \tfrac{1}{2}\delta(g) \tag{A.2.11}$$

where we used (A.2.3).
Choosing $\alpha = \frac{1}{2}(\sup g + \inf g)$ and plugging it in equation (A.2.7) we obtain

$$\begin{aligned}
\mathrm{Var}_{\mu}(g) &\leq \int \left(g - \tfrac{1}{2}(\sup g + \inf g)\right)^2 \, d\mu \\
&\leq \int \left(\tfrac{1}{2}\delta(g)\right)^2 \, d\mu \leq \tfrac{1}{4}\delta(g)^2 \; .
\end{aligned} \tag{A.2.12}$$

Thus, for a discrete metric we have

$$\begin{aligned}
\tfrac{1}{2}\|\mu-\nu\|_1 = R(\mu,\nu) &= \sup_f \frac{\left|\int f d\mu - \int f d\nu\right|}{\delta(f)} \\
&\leq \sup_f \left\{ \frac{\mathrm{Var}_{\mu}(f)^{\frac{1}{2}} \mathrm{Var}_{\mu}(g)^{\frac{1}{2}}}{\delta(f)} \right\} \\
&= \frac{1}{4}\delta(g) \; .
\end{aligned} \tag{A.2.13}$$

Therefore, recalling definition (A.1.4),

$$\begin{aligned} b_k &= \tfrac{1}{2} \int \|\mu_k(\cdot|x) - \nu_k(\cdot|x)\| \nu(dx) \\ &\leq \tfrac{1}{4} \delta_k(g) \int \left[\int g \; d\mu(\cdot|x) \right]^{-1} g(x) \mu(dx) \\ &= \tfrac{1}{4} \delta_k(g) \end{aligned} \tag{A.2.14}$$

hence, the estimate (A.1.5) becomes

$$\left| \mathrm{Cov}_\mu(f,g) \right| \leq \sum_i \sum_k b_k D_{ki} \delta_i(f) \leq \tfrac{1}{4} \sum_{i,k} \delta_i(f) \; D_{ki} \; \delta_k(g)$$

which completes the proof of Theorem 2.7.2.

Appendix B

Listings

We set out the final versions of the codes used for the numerical analysis presented in Chapter 3. First the C-CUDA code for the computation of the PCA-TASEP's coalescence times and then, the code in Ruby for the comparison of the Kac-Ising reversible and irreversible coalescence times.

B.1 CUDA PCA-TASEP Simulator

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include "cuda.h"
#include "driver_types.h"
#include "cuComplex.h"
// #include "cudadebug.h"
#include <curand.h>

// Ring reassignment
int new_ring(int L, float *s1, float *s2){
  size_t i;
  for( i = 1; i < L/2; i++ ){
  s1[i] = 0.0;
  }
  for( i = L/2; i < L; i++){
  s1[i] = 1.0; //check!
  }
// Shuffle balls from position 1 to L-1
  for (i = 1; i < L-1 ; i++) {
    int w =  i + (rand()/(RAND_MAX / (L-1 - i) + 1));
    float t = s1[w];
    s1[w] = s1[i];
    s1[i] = t;
  }
  s2[0] = 1.0;
  s2[1] = 0.0;
  for (i = 1; i < L-1; i++){
    s2[i] = s1[i];
  }
}
```

```
32
33 // Initialization
34 int iniz_coupling(int n, int L, float *h_v1, float *h_v2, float *h_c,
       float *h_CT, float *CTdistribution, int CTlength){
35   float *s;
36   s = (float*)malloc(L*sizeof(float));
37
38   size_t i;
39   for( i = 1; i < L/2; i++ ){
40   s[i] = 0.0;
41   }
42   for( i = L/2; i < L; i++){
43   s[i] = 1.0;
44   }
45   int k;
46   int j = 0;
47   for (k = 0; k < n; k++){
48     if (k%L == 0){
49       h_v1[k] = 0;
50       h_v2[k] = 1;
51     }
52     else if (k%L == L-1){
53       h_v1[k] = 1;
54       h_v2[k] = 0;
55     }
56     else{
57       h_v1[k] = s[k%L];
58       h_v2[k] = s[k%L];
59     }
60 // Shuffle balls from position 1 to L-1
61     if(k!=0 && k%L == 0){
62       for (i = 1; i < L-1 ; i++) {
63         int w =  i + (rand()/(RAND_MAX / (L-1 - i) + 1));
64         float t = s[w];
65         s[w] = s[i];
66         s[i] = t;
67       }
68     }
69   }
70 // Initialize the check_coalescence_vector: h_c for the difference v1-v2,
       h_CT and CTdistribution for the Coalescence Times
71   for (i = 0; i < n; i++){
72     h_c[i] = 0;
73   }
74   for (i = 0; i < n/L; i++){
75     h_CT[i] = 0;
76   }
77   for (i = 0; i < CTlength; i++){
78     CTdistribution[i] = 0;
79   }
80 }
81
82 // Deprecated sequential RNG
83 int sequential_randomvect(int n, double *vrnd){
84   size_t i;
85   for(i = 0; i < n; i++){
86     vrnd[i] = ((double)rand()/(double)RAND_MAX);
87   }
88 }
89
90 // Kernel functions
```

```
91  __global__ void compute_u(int n, int L, float *v1, float *u1, float *v2,
        float *u2, float *vrnd, float p){
92    int id = blockIdx.x*blockDim.x+threadIdx.x;
93
94    if (id < n){
95      if(v1[id%n] == 1){
96        if(v1[  L*(id/L) + (id+1)%L  ] == 0){
97          if ( vrnd[id] < p ){
98            u1[id] = -1;
99            u1[ L*(id/L) + (id+1)%L  ] = 1;
100         }
101       }
102     }
103
104     if(v2[id%n] == 1){
105       if(v2[  L*(id/L) + (id+1)%L  ] == 0){
106         if ( vrnd[id] < p ){
107           u2[id] = -1;
108           u2[ L*(id/L) + (id+1)%L  ] = 1;
109         }
110       }
111     }
112
113   }
114 }
115
116 __global__ void update_v(int n, int L, float *v1, float *u1, float *v2,
        float *u2){
117   int id = blockIdx.x*blockDim.x+threadIdx.x;
118
119   if (id < n){
120     v1[id] = v1[id] + u1[id];
121     v2[id] = v2[id] + u2[id];
122     u2[id] = 0;
123     u1[id] = 0;
124   }
125 }
126
127 __global__ void check_coalescence(int n, int L, float *v1, float *v2,
        float *c){
128   int id = blockIdx.x*blockDim.x+threadIdx.x;
129
130   // Evaluates the absolute difference between v1 and v2
131   if( id < n && id%L == 0){
132     for (int i = id; i < (id+L); i++){
133       c[i] = abs(v1[i]-v2[i]);
134     }
135   // Puts on the first element the total of the differences
136     for (int i = id+1; i < (id+L); i++){
137       c[id] = c[id] + c[i];
138     }
139   }
140 }
141
142 // Input parameters validation
143 void check_input(int n, int L, float p, float e, int nsteps, int step, int
        print_state){
144   if(n%L != 0){
145     printf("Error: the multi-ring must be a multiple of the size of the
        single ring!\n");
146     exit(0);
147   }
```

```
148   else if( p < 0 || p > 1){
149     printf("Error: the jump probability must be between 0 and 1\n");
150     exit(0);
151   }
152 }
153
154 // Needed just for quicksort
155 int compare (const void * a, const void * b)
156 {
157   return ( *(int*)a - *(int*)b );
158 }
159
160 int main( int argc, char* argv[] )
161 {
162 // Number of positions on the multi-ring
163   int n = 20000;
164 // Number of positions on the single ring
165   int L = 40;
166 // Lenght of the CTdistribution
167   int CTlength = 100000;
168 // Step for the evaluation of the coalescence
169   int step = 4;
170 // Step for the printing of the state
171   int print_state = 1;
172
173   float p = 0.7; // If I put (2L)^-1 I get a serial TASEP
174   float e = 0.0;
175
176 check_input(n, L, p, e, nsteps, step, print_state);
177
178 // Input vectors
179   float *h_v1, *d_v1, *s1;
180   float *h_u1, *d_u1;
181   float *h_v2, *d_v2 ,*s2;
182   float *h_u2, *d_u2;
183   float *h_vrnd, *d_vrnd;
184   float *h_coalescence, *d_coalescence;
185 // This vector will contain the value of the last iteration where it was
      found coalescence
186 // between two rings, value needed to correctly compute reassigned rings
      coalescence times
187   float *h_CT;
188   float *CTdistribution;
189
190 // Size, in bytes, of each vector
191   size_t bytes = n*sizeof(float);
192
193 // Allocate memory for each vector on host
194   h_v1 = (float*)malloc(bytes);
195   h_u1 = (float*)malloc(bytes);
196
197   h_v2 = (float*)malloc(bytes);
198   h_u2 = (float*)malloc(bytes);
199
200   s1 = (float*)malloc(bytes);
201   s2 = (float*)malloc(bytes);
202
203   h_vrnd = (float*)malloc(bytes);
204   h_coalescence = (float*)malloc(bytes);
205   h_CT = (float*)malloc((n/L)*bytes);
206
207   CTdistribution = (float*)malloc(CTlength*bytes);
```

```
208
209   curandGenerator_t gen;
210   curandCreateGenerator(&gen, CURAND_RNG_PSEUDO_DEFAULT);
211   curandSetPseudoRandomGeneratorSeed(gen, 1234ULL);
212
213 // When a ring coalescence the iteration is stored and the configuration
214 // is reassigned to check another ring configuration
215 for(L = 16; L <= 32; L += 4){
216   n = 1000*L;   // This can be obviusly adjusted according to hardware
        capability
217
218   iniz_coupling(n, L, h_v1, h_v2, h_coalescence, h_CT, CTdistribution,
        CTlength);
219   // sequential_randomvect(n, h_vrnd);
220
221   size_t i;
222   // for(i=0; i<n;i++){
223   //   if (i != 0 && i%L == 0 ){printf("\t");}
224   //   printf("%f ",h_vrnd[i]);
225   // }
226   // printf("\nCoupling vectors initialized!\n");
227   //  printf("\nh_v1\nh_v2\n");
228   //  for(i=0; i<n;i++){
229   //    if (i != 0 && i%L == 0 ){printf("\t");}
230   //    printf("%.0f ", h_v1[i]);
231   //  }
232   //  printf("\n");
233   //  for(i=0; i<n;i++){
234   //    if (i != 0 && i%L == 0 ){printf("\t");}
235   //    printf("%.0f ", h_v2[i]);
236   //  }
237   //  printf("\n\n");
238   //  update(n, L, h_v, h_vrnd, p, e);
239
240   // Allocate memory for each vector on GPU
241   cudaMalloc(&d_v1, bytes);
242   cudaMalloc(&d_u1, bytes);
243   cudaMalloc(&d_v2, bytes);
244   cudaMalloc(&d_u2, bytes);
245   cudaMalloc(&d_vrnd, bytes);
246   cudaMalloc(&d_coalescence, bytes);
247   // cudaCheckError("Error from first malloc");
248
249   // Copy the input data on the GPU
250   cudaMemcpy(d_v1, h_v1, bytes, cudaMemcpyHostToDevice);
251   cudaMemcpy(d_u1, h_u1, bytes, cudaMemcpyHostToDevice);
252   cudaMemcpy(d_v2, h_v2, bytes, cudaMemcpyHostToDevice);
253   cudaMemcpy(d_u2, h_u2, bytes, cudaMemcpyHostToDevice);
254   cudaMemcpy(d_coalescence, h_coalescence, bytes, cudaMemcpyHostToDevice);
255   // cudaMemcpy(d_vrnd, h_vrnd, bytes, cudaMemcpyHostToDevice);
256
257   int blockSize, gridSize;
258   // Number of threads in each thread block
259   blockSize = 512;
260   // Number of thread blocks in grid
261   gridSize = ((n+blockSize-1)/blockSize);
262   //  fprintf(stderr,"Bytes: %d blockSize %d griidSize %d\n",bytes,
        blockSize,gridSize);
263   // Execute the kernel
264   size_t j = 0;
265   size_t position = 0;
266
```

```
267   while(position < CTlength){
268     curandGenerateUniform(gen, d_vrnd, n);
269     compute_u<<<gridSize, blockSize>>>(n, L, d_v1, d_u1, d_v2, d_u2,
      d_vrnd, p);
270     update_v<<<gridSize, blockSize>>>(n, L, d_v1, d_u1, d_v2, d_u2);
271     check_coalescence<<<gridSize, blockSize>>>(n, L, d_v1, d_v2,
      d_coalescence);
272     // cudaCheckError("Error in update kernel");
273
274   // Build the Coalescence time statistics every 'step' iterations
275     if (j != 0 && j%step == 0){
276       size_t w = 0;
277       cudaMemcpy( h_coalescence, d_coalescence, bytes,
      cudaMemcpyDeviceToHost );
278
279       for(int q = 0; q < n/L; q++){
280   // If the first position of the diff vector is 0 and the corresponding
      element on CT
281   // vector isn't already filled, writes the actual iteration on it
282         if (h_coalescence[q*L] == 0){ // && h_CT[q] == -1 ){
283     // When a ring reach coalescence a new ring configuration is created
284           new_ring(L,s1,s2);
285           // printf("\nq = %d",q);
286       // Display the new ring configuration to reassign to the device
287
288           // printf("\ns1\t");
289           // for(w=0; w<L;w++){
290           // printf("%.0f ", s1[w]);
291           // }
292           // printf("\ns2\t");
293           // for(w=0; w<L;w++){
294           //   printf("%.0f ", s2[w]);
295           // }
296       //  The output vector is updated with the difference between the
      last coalescence time
297       //  of the old ring and the new one
298           CTdistribution[position] = j-h_CT[q];
299           // printf("\nposition = %d\n", position);
300           position++;
301           h_CT[q] = j;
302           // printf("\nh_CT\t");
303           // for(w = 0; w < n/L; w++){
304           //   printf("%.0f ", h_CT[w]);
305           // }
306           // printf("\nCTdistribution\t");
307           // for (w = 0; w < CTlength; w++){
308           //   printf("%.0f ", CTdistribution[w]);
309           // }
310       // The new ring configuration is copied on the device's arrays d_v1
      and d_v2
311       // with an offset equal to the beginning of the coalesced ring: q*L
312           cudaMemcpy(d_v1 + q*L, s1, L*sizeof(float),
      cudaMemcpyHostToDevice);
313           cudaMemcpy(d_v2 + q*L, s2, L*sizeof(float),
      cudaMemcpyHostToDevice);
314         }
315       }
316     }
317
318   // Print state and coalescence vectors every tot iterations, to control
      the update-----
319     // if (j!=0 && j%print_state == 0){
```

```
320     //   cudaMemcpy( h_v1, d_v1, bytes, cudaMemcpyDeviceToHost );
321     //   cudaMemcpy( h_v2, d_v2, bytes, cudaMemcpyDeviceToHost );
322     //   cudaMemcpy( h_coalescence, d_coalescence, bytes,
        cudaMemcpyDeviceToHost );
323     //   cudaMemcpy( h_vrnd, d_vrnd, bytes, cudaMemcpyDeviceToHost );
324     //   cudaCheckError("Error memcpy2");
325
326     //   size_t w = 0;
327
328       // printf("\n");
329       // for(w=0; w<n;w++){
330       //   if (w != 0 && w%L == 0 ){printf("\t");}
331       //   printf("%.0f ", h_v1[w]);
332       // }
333       // printf("\n");
334       // for(w=0; w<n;w++){
335       //   if (w != 0 && w%L == 0 ){printf("\t");}
336       //   printf("%.0f ", h_v2[w]);
337       // }
338       // printf("\nend of iteration \t%d of %d \t %.0f %% \n",j, nsteps,j
        *100.0/nsteps);
339     // }
340   // ------------------------------------------------------------
341     j++;
342   }
343
344   // Print the final CT vector: the array of instants when the coupled
        rings reach coalescence
345   printf("\nEnd of execution with L = %d", L);
346
347   FILE *f = fopen("results.txt", "a+");
348   if (f == NULL)
349   {
350     printf("\nError opening file!\n");
351     exit(1);
352   }
353
354   qsort(CTdistribution, CTlength, sizeof(float), compare);
355   fprintf(f, "\nring_length_%d,",L);
356   for (i = 0; i < CTlength; i++){
357     // printf("%.0f ", CTdistribution[i]);
358     fprintf(f, "%0.f,", CTdistribution[i]);
359   }
360   fclose(f);
361 }
362
363   printf("\n");
364   /* Cleanup */
365   curandDestroyGenerator(gen);
366   cudaFree(d_vrnd);
367   free(CTdistribution);
368   free(h_CT);
369
370   return EXIT_SUCCESS;
371 }
```

B.2 Kac-Ising Simulator

```ruby
#!/usr/bin/env ruby
require 'pry'
require 'matrix'
require 'ruby-progressbar'
require 'parallel'
require 'fileutils'
# require 'json'
# require 'descriptive_statistics'
# require_relative 'util'


def initsigma_sign(sign = 1)
  sign = sign/sign.abs   # returns only the sign of the argument
  conf = Array.new(@vol){sign}
  return conf
end

def initsigma_unif
  # initialize a uniform random configuration of +1 and -1
  segment = Random.new.rand(@vol)
  conf = Array.new(segment){1}
  conf += Array.new(@vol-segment){-1}
  return conf.shuffle!
end

# ------------------------------------ LOCAL FIELD
def m_irrev(i, conf)
  # empirical magnetization in i+1, i+1/gamma
  m = 0
  @gamma_inv.to_i.times do |j|
    m += conf[(i+1+j) % @vol]
  end
  m*(1.0/@gamma_inv)
end

def m_rev(i, conf)
  # empirical magnetization in i+1, i+1/gamma
  m = 0
  (@gamma_inv).to_i.times do |j|
    m += conf[(i-1-j) % @vol]
  end
  (@gamma_inv).to_i.times do |j|
    m += conf[(i+1+j) % @vol]
  end
  m*(1.0/(2*@gamma_inv))
end

# ------------------------------------ UPDATE RULES
def hb_update(s,i,p,m)
  b = @beta
  # Heat bath
  if p < Math.exp(b*m)/(2*Math.cosh(b*m))
    s[i] = 1
  else
    s[i] = -1
  end
end

def mod_update_rev(s,t,i,p)
```

```
60    if s[i] == -t[i]
61      t[i] = -t[i] if p > (1-Math.exp(-2*@beta*(m_rev(i,t)*t[i] + @a)))
62    else
63      t[i] = -t[i] if p < Math.exp(-2*@beta*(m_rev(i,t)*t[i] + @a))
64    end
65    s[i] = -s[i] if p < Math.exp(-2*@beta*(m_rev(i,s)*s[i] + @a))
66  end
67
68  def mod_update_irrev(s,t,i,p)
69    if s[i] == -t[i]
70      t[i] = -t[i] if p > (1-Math.exp(-2*@beta*(m_irrev(i,t)*t[i] + @a)))
71    else
72      t[i] = -t[i] if p < Math.exp(-2*@beta*(m_irrev(i,t)*t[i] + @a))
73    end
74    s[i] = -s[i] if p < Math.exp(-2*@beta*(m_irrev(i,s)*s[i] + @a))
75  end
76  # ------------------------------------ SAVE
77  def save_mix_times(ary)
78    folder = ".output/"
79    FileUtils.mkdir_p folder unless File.exists?(folder)
80
81    file_name = "L_#{@vol}-G_#{@gamma_inv.to_i}-B_#{@beta}.dat"
82
83    if File.exists?(folder+file_name)
84      old_data = File.read(folder+file_name).split("\n").map{|row|
85        row.split("\t").map{|x| x.to_i}}.transpose
86      new_data = [(old_data[0] + ary[0]).sort, (old_data[1] + ary[1]).sort]
87
88      FileUtils.rm(folder+file_name)
89    else
90      new_data = ary
91    end
92
93    new_data.transpose.each do |row|
94      File.open(folder+file_name, "a") do |f|
95        f.puts(row.join("\t"))
96      end
97    end
98    return file_name
99  end
100 # ------------------------------------ COUPLING
101 def coupling_irrev
102   tau   = initsigma_sign(+1)
103   sigma = initsigma_sign(-1)
104
105   rnd = Random.new(Random.new_seed)
106   pos = Random.new(Random.new_seed)
107
108   t = 0
109   while true do
110     p = rnd.rand
111     i = pos.rand(@vol)
112
113     # hb_update(sigma,i,p,m_irrev(i,sigma))
114     # hb_update(tau,i,p,m_irrev(i,tau))
115     mod_update_irrev(sigma,tau,i,p)
116     t += 1
117
118     if (t% (@vol)) == 0
119       # print_coup(sigma,tau,t)
120       if Vector.elements(sigma) == Vector.elements(tau)
121         return t
```

```
122         break
123       end
124     end
125   end
126 end
127 
128 def coupling_rev
129   tau = initsigma_sign
130   sigma = initsigma_sign(-1)
131 
132   rnd = Random.new(Random.new_seed)
133   pos = Random.new(Random.new_seed)
134 
135   t = 0
136   while true do
137     p = rnd.rand
138     i = pos.rand(@vol)
139 
140     # hb_update(sigma,i,p,m_rev(i,sigma))
141     # hb_update(tau,i,p,m_rev(i,tau))
142     mod_update_rev(sigma,tau,i,p)
143     t += 1
144 
145     if (t% (@vol)) == 0
146       # print_coup(sigma,tau,t)
147       if Vector.elements(sigma) == Vector.elements(tau)
148         return t
149         break
150       end
151     end
152   end
153 end
154 
155 def coupling_rev_irrev(betas, volumes, gammas)
156   caption = "Parallel enumeration"
157 
158   betas.each do |beta|
159     @beta = beta
160     @a = 1 #+ Math.log(2)/(2*@beta) #for the coupling of the mod_dynamics
161 
162     volumes.each do |vol|
163       @vol = vol
164 
165       gammas.each do |gamma_inv|
166         @gamma_inv = gamma_inv
167 
168           caption = "  Rev L_#{@vol}-B_#{@beta}-G_#{@gamma_inv}"
169           rev_results = Parallel.map(1..@samples, progress: caption) do
170             coupling_rev
171           end
172 
173           rev_results.sort!
174           # rev_results[0] = "REV"
175 
176           caption = "Irrev L_#{@vol}-B_#{@beta}-G_#{@gamma_inv}"
177           irrev_results = Parallel.map(1..@samples, progress: caption) do
178             coupling_irrev
179           end
180           irrev_results.sort!
181 
182           # irrev_results[0] = "IRREV"
183           save_mix_times([rev_results, irrev_results])
```

```
184         puts
185       end # gamma cycle
186     end # volume cycle
187     puts "\n\n"
188
189   end # beta cycle
190 # data <- read.delim('L_50-G_4-B_1.0-samples_100.dat', header = T)
191 # attach(data)
192 # p1 <- hist(REV); p2 <- hist(IRREV); plot(p1, col=rgb(0,0,1,0.25));
193 # plot(p2, col=rgb(1,0,0,0.25), add=T)
194 end #EOF
195
196 # ------------------------------------------------------------
197 class Array
198   def cut(value = nil)
199     if block_given?
200       inject([[]]) do |results, element|
201         if yield(element)
202           results << []
203         else
204           results.last << element
205         end
206
207         return results
208       end
209     else
210       results, arr = [[]], self.dup
211       until arr.empty?
212         if (idx = arr.index(value))
213           results.last.concat(arr.shift(idx))
214           arr.shift
215           results << []
216         else
217           results.last.concat(arr.shift(arr.size))
218         end
219       end
220       return results
221     end
222   end
223 end
224 # ------------------------------------------------------------
225
226 def single_chain(iterations)
227   rnd = Random.new(Random.new_seed)
228   pos = Random.new(Random.new_seed)
229   s = initsigma_unif
230
231   iterations.times do
232     p = rnd.rand
233     i = pos.rand(@vol)
234
235     s[i] = -s[i] if p < Math.exp(-2*@beta*(m_irrev(i,s)*s[i] + @a))
236   end
237   return s
238 end
239
240 def smooth_block_mag(s,width,threshold)
241 binding.pry
242   block_mags=s.each_slice(width).to_a.map{|x| x.inject(:+)/width.to_f}
243   block_mags.map!{ |x| x > (1-threshold)  ? x=1  : x}
244   block_mags.map!{ |x| x < (-1+threshold) ? x=-1 : x}
245 binding.pry
```

```
246   return block_mags
247 end
248
249 def phase_len(res)
250   len = Array.new
251   res.each do |blocks|
252     blocks = blocks.cut{|x| x.abs != 1}.delete_if{|x| x.length == 0}
253     blocks.each do |block|
254       idx = Array.new
255       block.each_with_index do |b,i|
256         next if i==0
257         idx.push(i) if b!= block[i-1]
258       end
259       idx.push(block.length)
260       count = [idx[0]]
261       idx.each_with_index do |e,i|
262         next if i == 0
263         count.push(e-idx[i-1])
264       end
265       len.push(count)
266     end
267   end
268   return len.flatten!
269 end
270
271 def save1D(ary, filename="saved")
272   folder = ".output/"
273   FileUtils.mkdir_p folder unless File.exists?(folder)
274   # ary.each{|e| e.sort!}
275   ary.each do |e|
276     File.open(folder+filename, "a") {|f| f.puts(e)}
277   end
278 end
279
280
281 @samples = 20000
282
283 betas = [0.5,0.9,1.0,1.1,1.2,1.4]
284 volumes = [5000]
285 gammas = [6,4,2]
286
287 coupling_rev_irrev(betas, volumes, gammas)
```

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