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Metastable states of the Ising chain with Kawasaki dynamics

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Abstract. We consider a ferromagnetic Ising chain evolving under Kawasaki dynamics at zero temperature. We investigate the statistics of the blocking time, as well as various characteristics of the metastable configurations reached by the system, including the statistics of the final energy, the spin correlations, and the distribution of domain sizes. Results of extensive numerical simulations are compared with analytical predictions made for the *a priori* ensemble of all blocked configurations with equal weights. Qualitative differences are found, *e.g.* in the domain sizes, which are found to be neither statistically independent nor exponentially distributed.

PACS. 05.70.Ln Nonequilibrium and irreversible thermodynamics – 64.60.My Metastable phases – 75.40.Gb Dynamic properties

1 Introduction

Glassy dynamics is often described as motion in a complex energy landscape [1], with many valleys separated by barriers. Valleys usually appear as metastable states with a very long, or even infinite, lifetime. They have been given various definitions [2–5], which are not equivalent from a dynamical point of view [6]. One common feature of all these approaches is the exponential growth with the system size of the number of valleys at fixed energy density E:

$$\mathcal{N}(N;E) \sim \exp(N S_{\rm ap}(E)), \tag{1.1}$$

where $S_{\rm ap}(E)$ is the configurational entropy or complexity. The subscript 'ap' underlines the fact that each valley is counted with the same *a priori* weight in the mere combinatorial problem of evaluating the configurational entropy.

An important issue concerns the *dynamical* weight of valleys, defined as follows. Assuming the initial configuration be random, with which probability does the system land in a given valley? A simple answer is that valleys admit a statistical description, just as configurations at thermal equilibrium. Along this line of thought, the most natural hypothesis is that all the possible valleys are sampled with equal statistical weights, possibly with the constraint that the mean energy is fixed, so that the *a priori* entropy (1.1) is also the relevant quantity from a dynamical viewpoint. In other words, dynamical quantities can be evaluated in a typical valley. More generally, valleys could be sampled with non-uniform weights, given by a simple effective Hamiltonian. The other extreme situation is that either the size of its basin of attraction (or another kind of 'hidden' detail) really matters for every single valley, so that the statistics of valleys induced by the dynamics is highly non-trivial.

The idea that metastable configurations can admit an *a priori* description by means of a uniform ensemble seems to have been first formulated by Edwards [7], in the specific context of granular materials. Since then, a uniform measure over metastable configurations is sometimes referred to as an Edwards measure, and the hypothesis that such a statistical description holds is termed the 'Edwards hypothesis'. We shall come back in the Discussion to the relationship between the present work and the ideas put forward by Edwards.

The simplest *a priori* statistical description, *i.e.*, the uniform one, is known to apply to the nonequilibrium relaxational dynamics of some mean-field models, where valleys have been shown to be sampled with equal weights. As a consequence, the configurational temperature $T_{\rm ap}$ defined by

$$\frac{1}{T_{\rm ap}} = \frac{{\rm d}S_{\rm ap}}{{\rm d}E} \tag{1.2}$$

has a thermodynamical meaning. In particular, it coincides with the effective temperature involved in the generalized fluctuation-dissipation relation [5].

Leaving the realm of mean-field models for the more realistic situation of models with short-range interactions on finite-dimensional lattices, one-dimensional spin systems

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with zero-temperature dynamics provide an adequate setting for investigating the dynamical weights of valleys, and especially for checking whether they admit a simple *a priori* statistical description, such as the uniform one. Indeed, the blocked configurations reached by zero-temperature dynamics are truly metastable states with infinite lifetimes. In an earlier work [8] we have addressed this question for Ising chains evolving under irreversible zero-temperature dynamics, where each spin may flip at most once before a blocked state is reached. These dynamical models can be exactly mapped onto random sequential adsorption problems [9], for which analytical tools are available. In that relatively simple situation, we found qualitative differences between dynamical results and the prediction of the uniform *a priori* description.

In the present work we pursue the investigation of metastable states in Ising chains, by considering the richer and hopefully more realistic situation of zero-temperature Kawasaki (spin-exchange) dynamics [10]. We allow the rate W_0 of diffusion processes (constant-energy moves) to vary [11]. If the kinetic constraint $W_0 = 0$ is imposed [12], only irreversible processes are present [8]. For the unconstrained dynamics ($W_0 > 0$), where diffusion processes are allowed, the dynamics is partly reversible. Each spin only flips a finite number of times, before the system globally reaches a blocked state after a finite time. The statistics of this blocking time is studied in Section 2. We then investigate various observables in the blocked configurations reached by the dynamics, starting from a random non-magnetized initial configuration. The data of extensive numerical simulations, presented in Section 4, are compared with the predictions of the uniform *a priori* approach, derived in Section 3. Finally, some aspects of persistence, in particular the distribution of the number of flips of a given spin, are discussed in Section 5.

To be more specific, we consider a ferromagnetic chain of Ising spins $\sigma_n = \pm 1$, whose Hamiltonian reads

$$\mathcal{H} = -\sum_n \sigma_n \sigma_{n+1}. \tag{1.3}$$

In Kawasaki dynamics [10], only pairs of opposite spins may be flipped ($+- \leftrightarrow -+$), so that the magnetization is locally conserved.

For simplicity, we limit ourselves to Monte-Carlo dynamics with random sequential updating, and we assume that the flipping rate only depends on the energy difference $\delta\mathcal{H}$ involved in the proposed move. Any given pair of opposite spins thus has a probability $W_{\delta\mathcal{H}}$ of flipping per unit time, with

$$\delta\mathcal{H} = 2(\sigma_{n-1}\sigma_n + \sigma_{n+1}\sigma_{n+2}) \in \{-4, 0, 4\}.$$

The requirement of detailed balance with respect to the Hamiltonian (1.3) at temperature $T = 1/\beta$ yields a single condition,

$$\frac{W_4}{W_{-4}} = \mathrm{e}^{-4\beta},$$

upon the rates W_4, W_0, W_{-4}.

Table 1. Allowed moves in zero-temperature Kawasaki dynamics.

$\delta\mathcal{H}$	type	name	rate	moves
-4	irreversible	condensation	1	$-+-+ \to --++$
				$+-+- \to ++--$
0	reversible	diffusion	W_0	$++-+ \leftrightarrow +-++$
				$-+-- \leftrightarrow --+-$

We furthermore restrict ourselves to zero-temperature dynamics, hence $W_4 = 0$. We choose time units such that $W_{-4} = 1$, keeping W_0 as a free parameter. The allowed moves and the corresponding rates are listed in Table 1. The zero-temperature limits of the Metropolis and heat-bath rules correspond respectively to $W_0 = 1$ and $W_0 = 1/2$. Hereafter we focus our attention on the range $0 \leq W_0 \leq 1$.

2 Statistics of blocking time

Let us first recall that for the kinetically constrained model ($W_0 = 0$) a finite system consisting of N spins reaches a blocked configuration after a finite blocking time $T_N \sim \ln N$, which is the jamming time of the equivalent problem of random sequential adsorption of hollow trimers [8]. The blocked configurations are characterized by the property that the spin patterns $+-+-$ and $-+-+$ are absent. Equivalently, there are at most two consecutive unsatisfied bonds.

In the present case ($W_0 > 0$) the system still gets trapped in a blocked configuration. However the diffusive motion of free $+$ spins in domains of $-$ spins, and *vice versa*, is allowed. Each free spin will eventually be annihilated, by meeting either another free spin or one of the boundaries of the domain. Blocked configurations of Kawasaki dynamics are therefore characterized by the property that the patterns $+-+$ and $-+-$ are absent. Equivalently, isolated spins are absent, or unsatisfied bonds are isolated.

In order to understand the statistics of the blocking time T_N, we consider first the regime $W_0 \ll 1$, where the time scales of condensation and diffusion are well separated [11]. The fast part of the dynamics, which occurs with unit rate, is identical to the constrained dynamics considered in references [8,12]. For intermediate times of order $1 \ll t \ll 1/W_0$, the system is therefore approximately left in one of the final configurations of the constrained dynamics. The slow, diffusive part of the dynamics then takes place at rate $W_0 \ll 1$. The late stages of the dynamics are governed by large domains, on which a single free spin diffuses. We assume that such large domains, of size $L \gg 1$, occur with an exponentially small probability

$$f_{\mathrm{dif}}(L) \sim \exp(-L/\xi_{\mathrm{dif}}),$$

where $\xi_{\rm dif}$ is the relevant characteristic length. The spin diffusion constant reads $D = W_0$ in our units. For a random initial point, the survival probability is known [13] to decay as $S(t;L) \approx (8L/\pi^2)\exp(-\pi^2 W_0 t/L^2)$. The mean density of free spins at time t can therefore be estimated as

$$S(t) \approx \sum_L f_{\rm dif}(L) S(t;L) \sim \int_0^\infty \exp\left(-\frac{L}{\xi_{\rm dif}} - \frac{\pi^2 W_0 t}{L^2}\right) L\,{\rm d}L. \tag{2.1}$$

Evaluating the integral by the method of steepest descent, we thus obtain stretched exponential decay for the density of free spins:

$$S(t) \sim t^{1/2}\,\exp\left(-\frac{(W_0 t)^{1/3}}{A_{\rm dif}}\right), \tag{2.2}$$

with

$$A_{\rm dif} = \left(\frac{4\xi_{\rm dif}^2}{27\pi^2}\right)^{1/3}. \tag{2.3}$$

This behavior, already emphasized in reference [11], is a general characteristic feature of diffusion processes in the presence of random traps [13]. The exponent 1/3 is related to the one-dimensional geometry; it would read $d/(d+2)$ for trapping problems in higher spatial dimension d. The above result should hold for the late stages ($W_0 t \gg 1$) of Kawasaki dynamics, for any finite value of W_0. The characteristic length $\xi_{\rm dif}$ is expected to depend smoothly on W_0.

For a finite system of N spins, the last free spin will be annihilated at a time T_N such that $NS(T_N) \sim 1$, hence $(W_0 T_N)^{1/3} \sim A_{\rm dif} \ln N$. More precisely, as the histories of spins diffusing on different domains are statistically independent, it can be argued along the lines of [8] that T_N is given according to extreme-value statistics [14] as

$$(W_0 T_N)^{1/3} \approx A_{\rm dif}\left(\ln\Big(N(\ln N)^{3/2}\Big) + b + X_N\right). \tag{2.4}$$

In this expression, the factor $(\ln N)^{3/2}$ takes account of the $t^{1/2}$ prefactor in the survival probability (2.2), while the effective constant b encompasses all subleading effects that have been neglected, and the random variable X_N is distributed according to the Gumbel law

$$f(X) = \exp(-X - {\rm e}^{-X}). \tag{2.5}$$

These predictions have been checked against extensive numerical simulations, performed according to the zero-temperature Kawasaki dynamics summarized in Table 1, with random sequential updates and periodic boundary conditions, starting from a random initial configuration with zero magnetization. The dynamics is run until the system gets trapped in a blocked configuration. The blocking time T_N is recorded for each sample. This measurement has been performed for many samples (10^8 spins in total for each value of W_0 and of N). The mean $\langle (W_0 T_N)^{1/3}\rangle$ is found to follow an almost perfect linear law when plotted against $\ln(N(\ln N)^{3/2})$, at least for N ranging from 50 to 3200, whereas the same data plotted against $\ln N$ are bent in a significant way. Using (2.3), the slope of the latter plot yields the value of the characteristic length $\xi_{\rm dif}$, which is plotted in Figure 1, against W_0. The error on this estimate, containing a systematic and a statistical part, is roughly comparable to the symbol size. The length $\xi_{\rm dif}$ exhibits a rather weak dependence on W_0, decreasing from $\xi_{\rm dif} = 1.77$ in the $W_0 \to 0$ limit to $\xi_{\rm dif} = 1.61$ for $W_0 = 1$.

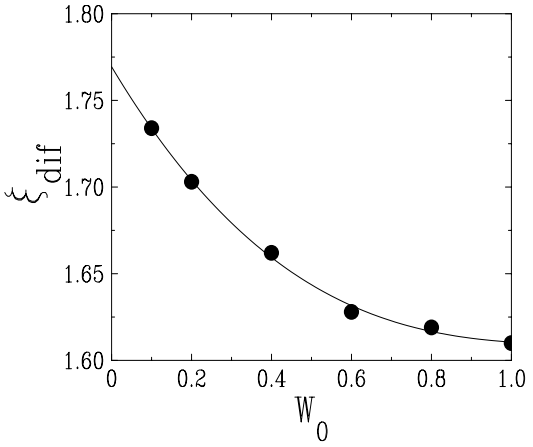

Fig. 1. Plot of the characteristic length $\xi_{\rm dif}$, extracted from the size dependence of $\langle (W_0 T_N)^{1/3}\rangle$, against the rate W_0. Symbols: numerical data. Errors are comparable to the symbol size. Line: third-degree polynomial fit.

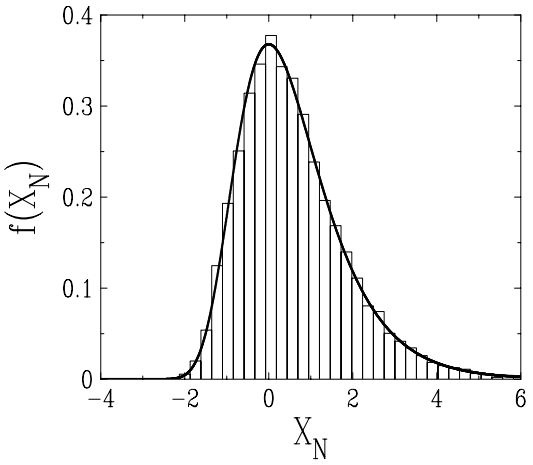

Fig. 2. Distribution of the variable X_N defined by (2.4). Histogram: numerical data for $N = 800$ (see text). Thick line: limit Gumbel law (2.5).

Another confirmation of the above picture is provided by Figure 2, showing a histogram plot of the variable X_N defined by (2.4), for 125,000 samples of size $N = 800$, with $W_0 = 1$. The parameter $A_{\rm dif} = 0.339$, *i.e.*, $\xi_{\rm dif} = 1.61$, is taken from the data of Figure 1, while the constant b is chosen by fitting the average $\langle X_N\rangle$. A convincing agreement is found with the limit law (2.5).

3 Blocked states: a priori ensemble

As already stated, the blocked states of zero-temperature Kawasaki dynamics are the configurations where isolated spins are absent. Equivalently, unsatisfied bonds are isolated.

This section is devoted to the statistical description of the blocked configurations taken with equal *a priori* weights. We shall distinguish the *full* ensemble of all the blocked configurations, irrespective of their energy, the *restricted* ensemble of blocked configurations with prescribed energy density E, and the *canonical* ensemble of blocked configurations, obtained by fixing the parameter β conjugate to the energy density E (see below).

3.1 Statistics of energy and configurational entropy

For a finite chain of N spins, we first investigate the number $\mathcal{N}(N;E)$ of blocked configurations with prescribed energy density E. This number can be evaluated by an elementary combinatorial reasoning [8]. For the sake of generality, we prefer to resort to the transfer-matrix formalism. We introduce the partition function $Z_N(\beta)$, defined as a sum over all the blocked configurations $\mathcal{C}=\{\sigma_n\}$ of the Boltzmann weight associated with the Hamiltonian (1.3). We have

$$Z_N(\beta)=\sum_{\mathcal{C}} \mathrm{e}^{-\beta\mathcal{H}(\mathcal{C})} \approx \int \mathcal{N}(N;E)\,\mathrm{e}^{-\beta N E}\,\mathrm{d}E. \quad (3.1)$$

In this framework, the parameter β can be positive or negative, and it is not related to physical temperature. The transfer matrix is then a very useful tool. Indeed the partition functions Z_N^{α}, labeled by the prescribed value $\alpha=(\sigma_{N-1},\sigma_N)$ of the last two spins, obey the recursion relation

$$\begin{pmatrix} Z_{N+1}^{++} \\ Z_{N+1}^{+-} \\ Z_{N+1}^{-+} \\ Z_{N+1}^{--} \end{pmatrix} = \mathcal{T} \begin{pmatrix} Z_{N}^{++} \\ Z_{N}^{+-} \\ Z_{N}^{-+} \\ Z_{N}^{--} \end{pmatrix},$$

where the 4×4 transfer matrix $\mathcal{T}$ reads

$$\mathcal{T}=\begin{pmatrix} \mathrm{e}^{\beta} & 0 & \mathrm{e}^{\beta} & 0 \\ \mathrm{e}^{-\beta} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathrm{e}^{-\beta} \\ 0 & \mathrm{e}^{\beta} & 0 & \mathrm{e}^{\beta} \end{pmatrix}.$$

The characteristic polynomial of $\mathcal{T}$ factors as $\det(\lambda\mathbf{1}-\mathcal{T})=(\lambda^2-\mathrm{e}^{\beta}\lambda-1)(\lambda^2-\mathrm{e}^{\beta}\lambda+1)$. The first (resp. the second) factor yields eigenvalues λ_1, λ_2 (resp. λ_3, λ_4), with

$$\lambda_{1,2}=\frac{1}{2}\left(\mathrm{e}^{\beta}\pm\sqrt{\mathrm{e}^{2\beta}+4}\right), \quad \lambda_{3,4}=\frac{1}{2}\left(\mathrm{e}^{\beta}\pm\sqrt{\mathrm{e}^{2\beta}-4}\right).$$

The left and right eigenvectors $\langle L_a|$ and $|R_a\rangle$ are even (resp. odd) for $a=1,2$ (resp. $a=3,4$) under the spin symmetry $+\leftrightarrow-$. We assume that they are normalized so that $\langle L_a|R_b\rangle=\delta_{ab}$. Their explicit expressions will not be needed hereafter.

For large N, we have $Z_N(\beta)\sim\lambda_1^N$, as λ_1 is the largest eigenvalue. Using (3.1), we obtain an exponential law of the form (1.1) for $\mathcal{N}(N;E)$, where the *a priori* configurational entropy $S_{\mathrm{ap}}(E)$ is related to $\ln\lambda_1(\beta)$ by a Legendre transform:

$$S_{\mathrm{ap}}(E)-\ln\lambda_1(\beta)=\beta E, \quad E=-\frac{\mathrm{d}\ln\lambda_1}{\mathrm{d}\beta}, \quad \beta=\frac{\mathrm{d}S_{\mathrm{ap}}}{\mathrm{d}E}.$$

Explicitly, we have

$$E=-\frac{\mathrm{e}^{\beta}}{\sqrt{\mathrm{e}^{2\beta}+4}}, \qquad \mathrm{e}^{\beta}=\frac{-2E}{\sqrt{1-E^2}}, \quad (3.2)$$

and the *a priori* entropy reads

$$S_{\mathrm{ap}}(E)=E\ln(-2E)+\frac{1-E}{2}\ln(1-E)-\frac{1+E}{2}\ln(1+E).$$

This entropy is non-zero for $-1<E<0$. It takes its maximal value

$$S^{\star}=\ln\Phi=0.481212,$$

where $\Phi=(1+\sqrt{5})/2$ is the golden mean, for

$$E^{\star}=-\frac{1}{\sqrt{5}}=-0.447214, \quad (3.3)$$

corresponding to $\beta=0$. Equation (3.3) therefore yields the typical *a priori* energy density of a blocked configuration.

The result (1.1) can be recast as follows. Consider the full ensemble of all the blocked configurations, irrespective of their energy. The probability of observing, in that ensemble, a blocked configuration with energy density E reads

$$P_{\mathrm{ap}}(E)\sim\exp\left(-N\Sigma_{\mathrm{ap}}(E)\right), \qquad \Sigma_{\mathrm{ap}}(E)=S^{\star}-S_{\mathrm{ap}}(E). \quad (3.4)$$

The function $\Sigma_{\mathrm{ap}}(E)$ vanishes quadratically as

$$\Sigma_{\mathrm{ap}}(E)\approx c\,(E-E^{\star})^2, \qquad c=\frac{5\sqrt{5}}{8}.$$

The bulk of the *a priori* distribution of E is therefore a narrow Gaussian around $E^{\star}$, whose rescaled variance asymptotically reads

$$N\,\mathrm{Var}\,E=N\left(\langle E^2\rangle-E^{\star\,2}\right)\underset{N\to\infty}{\longrightarrow}\frac{1}{2c}=\frac{4\sqrt{5}}{25}=0.357771.$$

The above results also allow to determine the higher cumulants of the energy in the canonical ensemble (at fixed parameter β). One has indeed

$$\frac{1}{N}\ln\left\langle \mathrm{e}^{sNE}\right\rangle_{\beta}=\frac{1}{N}\ln\frac{Z_N(\beta-s)}{Z_N(\beta)}\underset{N\to\infty}{\longrightarrow}\ln\frac{\lambda_1(\beta-s)}{\lambda_1(\beta)}.$$

By expanding this result as a power series in s, we obtain explicit expressions for the cumulants $\langle\!\langle E^k\rangle\!\rangle$ as a function of β.

As far as mean quantities are concerned, the microcanonical or restricted ensemble (fixed energy density E) and the canonical one (fixed conjugate parameter β) are equivalent. It is therefore justified to recast canonical results in terms of the prescribed value E of the mean energy, using (3.2). Generalizing this equivalence prescription to the cumulants of the energy, we obtain

$$\begin{aligned} N \operatorname{Var} E = N\langle\!\langle E^2 \rangle\!\rangle &\underset{N\to\infty}{\longrightarrow} -E(1-E^2), \\ N^2\langle\!\langle E^3 \rangle\!\rangle &\underset{N\to\infty}{\longrightarrow} -E(1-E^2)(3E^2-1), \\ N^3\langle\!\langle E^4 \rangle\!\rangle &\underset{N\to\infty}{\longrightarrow} -E(1-E^2)(15E^4-12E^2+1). \end{aligned} \tag{3.5}$$

The results (3.5) can be given the following interpretation. Fixing β amounts to fixing the extensive part NE of the energy, while the equivalence prescription is a natural ansatz to describe the fluctuations of its non-extensive part.

3.2 Spin correlation function

The spin correlation function $C_n = \langle \sigma_0 \sigma_n \rangle$ in the canonical *a priori* ensemble can also be evaluated by the transfer-matrix method. In the bulk of an infinitely long chain, and for $n \geq 0$, we have

$$C_n = \frac{\langle L_1 | \mathcal{S}\mathcal{T}^n \mathcal{S} | R_1 \rangle}{\lambda_1^n} = \sum_a \langle L_1 | \mathcal{S} | R_a \rangle \langle L_a | \mathcal{S} | R_1 \rangle \left(\frac{\lambda_a}{\lambda_1} \right)^n , \tag{3.6}$$

where

$$\mathcal{S} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

is the spin operator.

Because of symmetry, only the eigenvectors with $a = 3, 4$ contribute to the above sum. The values $C_0 = 1$ and $C_1 = -E$ allow to determine the products of matrix elements entering (3.6), without knowing the eigenvectors explicitly. The following alternative reasoning can also be used. Being a linear combination of $(\lambda_3/\lambda_1)^n$ and $(\lambda_4/\lambda_1)^n$, C_n can be shown to obey the three-term recursion relation

$$(1-E)C_{n+2} + 2EC_{n+1} + (1+E)C_n = 0.$$

The initial values $C_0 = 1$ and $C_1 = -E$ are therefore again sufficient to determine the correlation function for all values of the distance n.

For $-1/\sqrt{2} \leq E \leq 0$, which contains the range of final energies reached by the dynamics, $\lambda_{3,4} = \exp(\pm \mathrm{i} Q)$ are complex numbers with unit modulus, with

$$\tan Q = \frac{\sqrt{1-2E^2}}{-E} \qquad (0 \leq Q \leq \pi/2). \tag{3.7}$$

We are thus led to the expression

$$C_n = \left(\frac{1+E}{1-E} \right)^{n/2} \left(\cos nQ + \frac{E^2}{\sqrt{1-2E^2}} \sin nQ \right), \tag{3.8}$$

for $n \geq 0$. In the *a priori* ensemble, the spin correlation function therefore exhibits an exponential decay, of the form $\exp(-n/\xi_{\mathrm{spin}})$, modulated by oscillations at wavevector Q. Both the correlation length

$$\xi_{\mathrm{spin}} = \frac{2}{\ln \dfrac{1-E}{1+E}} \tag{3.9}$$

and the wavevector Q, given by (3.7), depend continuously on energy.

We finally quote for further reference the value of the reduced susceptibility

$$\widehat{\chi} = \sum_{n=-\infty}^{\infty} C_n. \tag{3.10}$$

After some algebra, we obtain the simple result

$$\widehat{\chi} = \frac{-E(1-E)}{1+E}. \tag{3.11}$$

3.3 Distribution of domain sizes

Another characteristic feature of blocked states is the distribution of domain sizes $f(\ell)$, defined as the probability that a given domain consists exactly of ℓ consecutive parallel spins. Since isolated spins are absent, domains have at least size two ($\ell \geq 2$).

In the *a priori* ensemble, the distribution $f(\ell)$ can again be evaluated by the transfer-matrix method. Indeed $\rho(\ell)$, the density (per unit length) of domains consisting of exactly ℓ spins, admits an expression similar to the middle side of (3.6), namely

$$\begin{aligned} \rho(\ell) &= \frac{\left\langle L_1 | \mathcal{P}\, \mathrm{e}^{(\ell-2)\beta} | R_1 \right\rangle}{\lambda_1^\ell} \\ &= \langle L_1 | \mathcal{P} | R_1 \rangle \ \frac{1+E}{1-E} \left(\frac{-2E}{1-E} \right)^{\ell-2}, \end{aligned}$$

where

$$\mathcal{P} = (|{+}{-}\rangle\langle{-}{+}|) + (|{-}{+}\rangle\langle{+}{-}|) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

is the appropriate domain boundary operator. The explicit expression of the matrix element is not needed, as it can be fixed by normalization. The probability distribution $f(\ell)$ of domain sizes indeed reads $f(\ell) = \rho(\ell)/\rho$, where ρ is the total density of domains (or equivalently, of domain walls).

We thus obtain the geometric (*i.e.*, discrete exponential) probability distribution

$$f(\ell) = \frac{1+E}{1-E}\left(\frac{-2E}{1-E}\right)^{\ell-2} \tag{3.12}$$

for $\ell \geq 2$, and consistently

$$\rho = \sum_{\ell=2}^{\infty} \rho(\ell) = \frac{1}{\langle \ell \rangle} = \frac{1+E}{2} = \langle L_1 | \mathcal{P} | R_1 \rangle \cdot \tag{3.13}$$

The characteristic length of (3.12),

$$\xi_{\rm dom} = \frac{1}{\ln \dfrac{1-E}{-2E}}, \tag{3.14}$$

is in general different from the spin correlation length $\xi_{\rm spin}$ of (3.9), except for the typical value of energy (3.3), where $\xi_{\rm spin} = \xi_{\rm dom} = 1/S^\star$.

The mean of the domain size distribution (3.12) agrees with (3.13), while its variance reads

$$\mathrm{Var}\,\ell = \sum_{\ell=2}^{\infty} \ell^2 f(\ell) - \langle \ell \rangle^2 = \frac{-2E(1-E)}{(1+E)^2}\cdot$$

Consider now a large sample of N spins, in the canonical *a priori* ensemble (fixed parameter β). The number M of domains in the sample is such that $N = \ell_1 + \cdots + \ell_M$ is the sum of M independent variables distributed according to $f(\ell)$, neglecting boundary effects. The expected number of domains and its variance are given by

$$\begin{aligned} \frac{\langle M \rangle}{N} &\underset{N\to\infty}{\longrightarrow} \frac{1}{\langle \ell \rangle} = \frac{1+E}{2}, \\ \frac{\mathrm{Var}\,M}{N} &\underset{N\to\infty}{\longrightarrow} \frac{\mathrm{Var}\,\ell}{\langle \ell \rangle^3} = \frac{-E(1-E^2)}{4}\cdot \end{aligned} \tag{3.15}$$

One has therefore

$$N\,\mathrm{Var}\,E = \frac{4\,\mathrm{Var}\,M}{N} \underset{N\to\infty}{\longrightarrow} \frac{4\,\mathrm{Var}\,\ell}{\langle \ell \rangle^3}, \tag{3.16}$$

so that the second result of (3.15) agrees with expression (3.5) for $N\,\mathrm{Var}\,E$.

4 Blocked states: dynamics

In this section we compare the predictions of the *a priori* approach, derived in Section 3, to the results of numerical simulations concerning the blocked configurations reached by the dynamics. We have used the rules of the zero-temperature Kawasaki dynamics summarized in Table 1, with random sequential updates, starting from a random non-magnetized initial configuration.

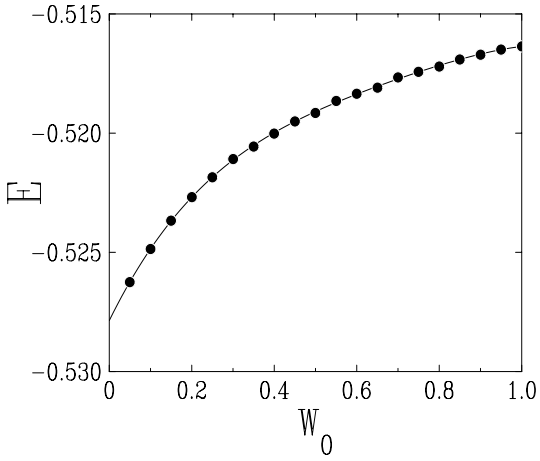

Fig. 3. Plot of the mean final energy E against the rate W_0. Symbols: numerical data. Statistical errors are smaller than the symbol size. Line: fifth-degree polynomial fit, yielding the extrapolated value (4.3) in the $W_0 \to 0$ limit.

4.1 Mean energy

The first and the simplest quantity to be measured is the mean energy E of the blocked configurations reached by the dynamics.

Let us start with a reminder of the kinetically constrained model ($W_0 = 0$). For a random initial configuration, the two kinds of allowed defects, namely isolated unsatisfied bonds (domain walls) and domains of two unsatisfied bond (isolated spins) occur respectively with the following densities in blocked configurations [8,12]:

$$\begin{aligned} q_1 &= \frac{1}{2}\left(1 - \mathrm{e}^{-5/4} - \mathrm{e}^{-9/4}\int_1^{3/2} \mathrm{e}^{y^2}\,\mathrm{d}y\right) = 0.219704, \\ q_2 &= \frac{\mathrm{e}^{-5/4}}{4} = 0.071626, \end{aligned} \tag{4.1}$$

so that the mean energy of blocked configurations reads

$$E_0 = -1 + 2q_1 + 4q_2 = -\mathrm{e}^{-9/4}\int_1^{3/2} \mathrm{e}^{y^2}\,\mathrm{d}y = -0.274087. \tag{4.2}$$

In the present case ($W_0 \neq 0$), the mean energy E of blocked states is expected to be below this number. Indeed the diffusive moves can only help relaxing more efficiently the energy excess of the disordered initial state.

Figure 3 shows a plot of the mean final energy E against the diffusive rate W_0. Each data point corresponds to 10^8 spins in total. We have checked that no appreciable size dependence is to be observed. The final energy is found to be well below (4.2), and below the typical *a priori* value (3.3). It only exhibits a very weak dependence on the rate W_0, increasing from the extrapolated minimum value

$$E(0) = -0.5279 \tag{4.3}$$

Table 2. First four scaled cumulants of the energy of the blocked configurations. Comparison between numerical results and predictions of the full and restricted *a priori* ensembles (see text).

scaled cumulant	numerical result	full *a priori*	restricted *a priori*
$\langle\langle E \rangle\rangle = E$	-0.51633	-0.44721	-0.51633
$N\langle\langle E^2 \rangle\rangle = N \operatorname{Var} E$	0.3446	0.35777	0.37868
$N^2\langle\langle E^3 \rangle\rangle$	0.031	-0.14311	-0.07582
$N^3\langle\langle E^4 \rangle\rangle$	-0.46	-0.28622	-0.42906

in the $W_0 \to 0$ limit to the maximum value

$$E(1) = -0.51633 \tag{4.4}$$

for $W_0 = 1$.

The regime $W_0 \ll 1$ again deserves some more attention. The mean energy has a discontinuity at $W_0 = 0$. Indeed the $W_0 \to 0$ limit of the energy, $E(0)$ given by (4.3), is different from that of the constrained dynamics, E_0 given by (4.2). This discontinuity can be analyzed as follows. In the diffusive part of the dynamics, free spins annihilate by meeting either each other or domain walls. The collision of a single free spin with a domain wall relaxes 4 units of energy, while the coalescence between $n \geq 2$ spins within a domain relaxes $4(n-1)$ units of energy, *i.e.*, $4(n-1)/n$ per spin. If all the free spins were annihilated in meeting domain walls, the final energy would assume the value $E = E_0 - 4p_2$. The efficiency of the diffusive relaxation mechanism can therefore be characterized by the ratio

$$\eta = \frac{E_0 - E(0)}{4p_2} = 1 - \sum_{n \geq 2} \frac{\Pi_n}{n},$$

where Π_n is the probability that a given free spin gets annihilated in a coalescence of $n \geq 2$ spins. The extrapolated value (4.3) of the final energy yields a rather high efficiency: $\eta = 0.886$.

In view of the weak dependence of the final energy on the rate W_0 (see Fig. 3), hereafter we restrict the numerical analysis to the case $W_0 = 1$ of zero-temperature Metropolis dynamics.

4.2 Higher cumulants of energy

We now turn to the statistics of the energy of the blocked configurations, besides its mean value studied above. In analogy with the *a priori* estimate (3.4), the final energy is expected to obey a large-deviation formula of the type

$$P(E) \sim \exp(-N\Sigma(E)),$$

with $\Sigma(E)$ being the dynamical entropy. This formula implies that the cumulants of the total energy scale as $\langle\langle (NE)^k \rangle\rangle \sim N$, just as in usual equilibrium situations.

Instead of measuring the whole function $\Sigma(E)$, which would require a quite extensive numerical effort, we have measured the first four cumulants of the energy of the blocked configurations. Table 2 gives the measured values of the scaled energy cumulants for $W_0 = 1$ and a random initial configuration. For comparison we also list the predictions of the full *a priori* ensemble (3.5) for $E = E^\star$ of (3.3), and of the restricted *a priori* ensemble, obtained by inserting into (3.5) the observed value (4.4) of the mean energy. The simulations have been performed on samples of various sizes ranging from $N = 50$ to 200, having 10^{10} spins in total. No systematic size dependence is observed. Statistical errors can be estimated to be of the order of one unit of the least significant digit. Both *a priori* schemes perform very unequally in predicting the energy cumulants. The variance is rather accurately predicted by both schemes, which perform equally poorly for the third cumulant, while the restricted scheme is definitely better for the fourth cumulant.

4.3 Spin correlation function

We now turn to the spin correlation function $C_n = \langle \sigma_0 \sigma_n \rangle$ in the blocked configurations. This quantity has two remarkable properties. First, since isolated spins are not allowed in blocked configurations, we have $C_1 = 1 - 2\rho = -E$ and $C_2 = 1 - 4\rho$, where ρ is the density of domain walls (3.13), hence

$$C_2 = 2C_1 - 1. \tag{4.5}$$

Second, the total magnetization $M = \sum_n \sigma_n$ is exactly conserved in Kawasaki dynamics. Furthermore, for a homogeneous non-magnetized state, we have $\langle M^2 \rangle = N\widehat{\chi}$, with the definition (3.10). The quantity $\widehat{\chi}$ therefore has the same value in the initial and final configurations, *i.e.*, for a random initial state,

$$\widehat{\chi} = \sum_{n=-\infty}^{\infty} C_n = 1. \tag{4.6}$$

Figure 4 shows a comparison between numerical data (circles and full line), corresponding to 3×10^9 spins in total, and the prediction (3.8) of the restricted *a priori* ensemble at the observed mean energy (4.4) (triangles and dashed line). The *a priori* prediction and numerical data coincide both for $n = 1$ (by construction, as E has been imposed) and for $n = 2$ (as a consequence of (4.5)). For larger distances, the spin correlations oscillate in sign and fall off exponentially, in qualitative agreement with the

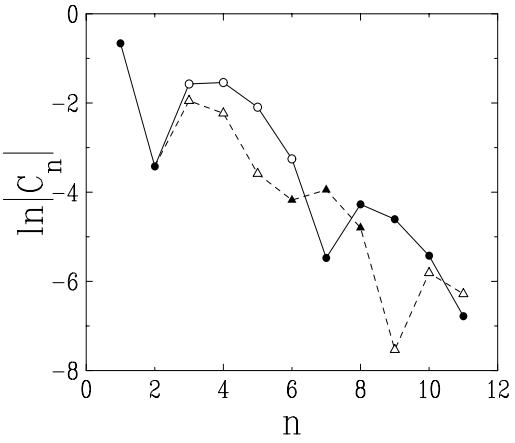

Fig. 4. Logarithmic plot of the absolute value of the spin correlation function $|C_n|$, against distance n. Full (open) symbols show positive (negative) correlations. Circles and full line: numerical data. Statistical errors are smaller than the symbol size. Triangles and dashed line: prediction (3.8) of restricted *a priori* ensemble at energy (4.4).

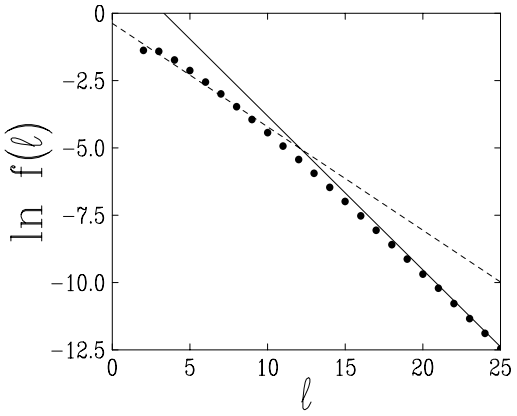

Fig. 5. Logarithmic plot of the probability distribution $f(\ell)$ against domain size ℓ. Circles: numerical data. Statistical errors are much smaller than the symbol size. Dashed straight line: prediction (3.12) of *a priori* ensemble at energy (4.4). Full straight line: guide to the eye with inverse slope $\xi_{\rm dom} = 1.75$.

a priori prediction. Both the period of oscillations and the decay length are observed to be slightly larger than those of the *a priori* ensemble. These observations remain however at a qualitative level. We also notice that the *a priori* ensemble fails to reproduce the identity (4.6). Indeed $\widehat{\chi}$ of (3.11) equals unity for $E = 1-\sqrt{2} = -0.414214$, a value which neither agrees with the most probable *a priori* energy $E^\star$ of (3.3), nor with the observed mean energy (4.4). Conversely, the prediction for the correlation function of the restricted *a priori* ensemble at energy (4.4), plotted in Figure 4, has $\widehat{\chi} = 1.6192$, which is significantly different from unity.

4.4 Distribution of domain sizes

We have determined the distribution of domain sizes $f(\ell)$ by means of extensive numerical simulations, with a random initial state. Figure 5 shows our data corresponding to 3×10^9 spins in total. The observed distribution is not exponential, at variance with the prediction (3.12) of the *a priori* ensemble. The full line suggests an exponential asymptotic fall-off of the distribution, with a characteristic length $\xi_{\rm dom} = 1.75$. This length is close to the characteristic length of domains with a single diffusive spin, $\xi_{\rm dif} = 1.61$, plotted in Figure 1. As a matter of fact, the equality $\xi_{\rm dom} = \xi_{\rm dif}$ is expected to hold in the $W_0 \to 0$ limit. The prediction (3.12) of the restricted *a priori* ensemble at the observed mean energy (4.4) is shown as a straight dashed line, whose inverse slope is the prediction $\xi_{\rm dom} = 2.603$ (3.14) of the *a priori* approach.

Another noticeable difference with the prediction of the *a priori* approach is that the sizes of successive domains in the final states of the dynamics are not independent. Indeed, if they were so, the relation (3.16) would hold, while the data yield $4\,{\rm Var}\,\ell/\langle\ell\rangle^3 = 0.2790$, a number significantly below the observed variance $N\,{\rm Var}\,E = 0.3446$, listed in Table 2. Hence domain sizes exhibit a weak but definite *positive* correlation. Domain sizes which are neither statistically independent nor exponentially distributed have also been observed recently [15] in spin chains undergoing tapping dynamics.

5 Features of persistence

We now turn to features related to the whole history of a single given spin, say σ_0, the spin situated at the origin. This kind of problems belongs to the realm of persistence. In the present context, the central quantity is ν, the total number of times σ_0 flips during the history of the sample, before a blocked configuration is reached. The number ν of spin flips is finite with unit probability in the limit of a large system. Zero-temperature Kawasaki dynamics is therefore of type $\mathcal{F}$ in the classification of [16]. Furthermore ν is random, as it depends both on the initial configuration and on the history of the system. We are therefore interested in the distribution p_ν of the number of flips, which is expected to have a well-behaved limit when σ_0 is deep inside a large enough sample.

Before presenting numerical data, we first predict the main salient features of the distribution p_ν, following the lines of Section 2. Consider again a large domain of $L \gg 1$ spins, containing the origin, on which a single free spin diffuses. The spin σ_0 flips twice each time the free spin traverses the origin. We are thus led to the following effective problem.

Consider a random walker in the interval $-L_1 < n < L_2$, with absorbing boundaries at $n = -L_1$ and $n = L_2$. The walker starts from the origin ($n = 0$). The probability that the walker returns to the origin before being absorbed by either boundary reads

$$P_{\rm ret}(L_1, L_2) = 1 - \frac{1}{2}\left(\frac{1}{L_1} + \frac{1}{L_2}\right)\cdot \qquad (5.1)$$

This formula relies on a well-known result in the gambler's ruin problem [17]. Indeed, suppose that the walker's first jump is to the right (resp. to the left), and consider $0 \leq n \leq L_2$ (resp. $0 \leq -n \leq L_1$) as the gambler's wealth. Then the ruin probability reads $P = 1 - 1/L_2$ (resp. $P = 1 - 1/L_1$). The expression (5.1) is the arithmetical mean of both ruin probabilities.

The probability that σ_0 flips an even number $\nu = 2k \gg 1$ of times therefore approximately reads $p_{2k}(L_1, L_2) \sim (P_{\rm ret}(L_1, L_2))^k (1 - P_{\rm ret}(L_1, L_2))$. Hence the distribution of the number of flips can be estimated, in analogy with (2.1), as

$$\begin{aligned} p_{2k} &\approx \sum_{L_1, L_2} (L_1 + L_2 - 1)\, f_{\rm dif}(L_1 + L_2 - 1) \\ &\quad \times P_{\rm ret}(L_1, L_2)^k (1 - P_{\rm ret}(L_1, L_2)) \\ &\sim \left(\int_0^\infty \exp\left(-\frac{L}{\xi_{\rm dif}} - \frac{k}{2L} \right) {\rm d}L \right)^2 . \end{aligned}$$

The integral entering this expression closely resembles that entering (2.1). For $k \gg 1$ it is legitimate to use the steepest-descent method. The saddle point lies at $L_c = \sqrt{k \xi_{\rm dif}/2}$. We thus obtain the stretched exponential law

$$p_{2k} \sim \sqrt{k}\, \exp\left(-2 \sqrt{\frac{2k}{\xi_{\rm dif}}} \right) \tag{5.2}$$

for the distribution of the number of spin flips, provided $\nu = 2k$ is a large even number.

The occurrence of odd numbers $\nu = 2k + 1$ of spin flips can also be explained in the above framework, if the spin σ_0 is either situated at an endpoint of a domain, or involved in a coalescence event between two free spins. Both effects are expected to scale as the inverse of the domain size L. This leads us to predict that odd values of ν are suppressed by a factor of order $1/L_c$, *i.e.*,

$$\frac{p_{2k+1}}{p_{2k}} \approx \frac{a}{\sqrt{k \xi_{\rm dif}}}. \tag{5.3}$$

Figure 6 shows a logarithmic plot of the distribution p_ν of the number of flips. The simulations again concern samples of various sizes having 2×10^{10} spins in total, with $W_0 = 1$. Even numbers of spin flips $\nu = 2k$ (full symbols) are clearly more frequent than odd numbers $\nu = 2k + 1$ (open symbols), especially for large values of k. From a quantitative viewpoint, the full lines on Figure 6 show a common fit of the numerical data for $\nu > 10$ according to the asymptotic predictions (5.2), (5.3). We thus obtain $2/\sqrt{\xi_{\rm dif}} \approx 1.55$, in agreement with the data of Figure 1, $\xi_{\rm dif} \approx 1.61$, *i.e.*, $2/\sqrt{\xi_{\rm dif}} \approx 1.57$. We also obtain $a \approx 1.5$, albeit with a large uncertainty.

Besides the above analysis of the regime of large numbers of spin flips, due to long surviving free spins, our data yield yet other interesting informations. First, the persistence probability, *i.e.*, the probability for a spin to never flip, has the following value:

$$p_0 = 0.44739.$$

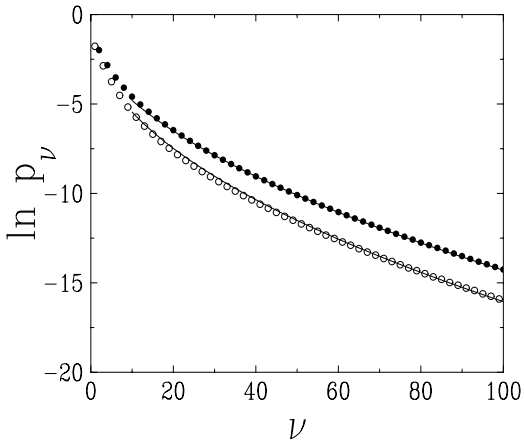

Fig. 6. Logarithmic plot of the distribution p_ν of number of flips. Full symbols: data for $\nu = 2k$ even. Open symbols: data for $\nu = 2k + 1$ odd. Statistical errors are much smaller than the symbol size. Full lines: common fit described in the text.

Then, the probability that a spin flips an even or an odd number of times reads

$$P_{\rm even} = \sum_{k \geq 0} p_{2k} = 0.72302,$$

$$P_{\rm odd} = \sum_{k \geq 0} p_{2k+1} = 1 - P_{\rm even} = 0.27698.$$

These figures can be related to the overlap between a random initial configuration and the corresponding final one. We have indeed

$$Q = \langle \sigma_0(0) \sigma_0(\infty) \rangle = \sum_{\nu \geq 0} (-1)^\nu p_\nu = P_{\rm even} - P_{\rm odd} = 0.44604.$$

The mean number of spin flips reads

$$\langle \nu \rangle = \sum_{\nu \geq 0} \nu\, p_\nu = 2.06916.$$

This quantity can be used to determine the fractions $f_{\rm cond}$ of condensation moves and $f_{\rm dif}$ of diffusive moves in a typical history, starting from a random initial configuration. Indeed, on the one hand, a condensation move lowers the total energy by four units, while a diffusive moves leaves it unchanged (see Tab. 1). On the other hand, any move involves exactly two spin flips. We have therefore, using (4.4),

$$f_{\rm cond} = 1 - f_{\rm dif} = -\frac{E}{2\langle \nu \rangle} = 0.12477.$$

To close up, let us compare the above results to the case of constrained Kawasaki dynamics ($W_0 = 0$) [8,12], where only condensation moves are allowed. In this situation, the above quantities can be simply related to the final energy E_0 of (4.2). Indeed every spin flips at most once, so that only p_0 and $p_1 = 1 - p_0$ are non-zero, and $f_{\rm cond} = 1$. Starting again from a random configuration, we are left with

$$2(1 - p_0) = 1 - Q = 2\langle \nu \rangle = -E_0 = 0.274087.$$

Table 3. Four different zero-temperature dynamics of the ferromagnetic Ising chain, with appropriate references (brackets).

conserved magnetization	diffusive moves	dynamics	behavior
no	yes	Glauber [18]	coarsening [19]
no	no	constrained Glauber [20]	metastability [8]
yes	yes	Kawasaki [10]	metastability [this work]
yes	no	constrained Kawasaki [12]	metastability [8]

6 Discussion

First, we wish to emphasize the richness of the zero-temperature dynamics of the ferromagnetic Ising chain. There are indeed four different natural kinds of dynamics, summarized in Table 3. Only Glauber dynamics gives rise to a bona fide coarsening dynamics, obeying dynamical scaling with a typical domain size growing as $L(t) \sim \sqrt{t}$. With the three other dynamics, the system is left in a metastable configuration after a relatively short blocking time. The constrained Glauber and Kawasaki dynamics have been analyzed in our previous work [8]. Each spin may flip at most once, before a global blocked state is reached. The blocking time scales with the number of spins as $\ln N$. These models can be exactly mapped onto the random sequential addition problem of dimers and hollow trimers, respectively, hence allowing an analytical treatment.

The last case not considered so far from the viewpoint of metastability, Kawasaki dynamics, has been the subject of this work. Because of the diffusive moves, the dynamics is only partly irreversible. This novel feature makes the Kawasaki problem both richer and hopefully closer to more realistic situations. The number of flips of a given spin, although finite with probability one, may be arbitrarily large. The blocking time grows as $(\ln N)^3$. On the other hand, analytical tools being no longer available, we needed to have recourse to numerical simulations.

First, we wish to underline that the description of the late stages of the zero-temperature Kawasaki dynamics in terms of an effective trapping problem for single free spins, already emphasized in reference [11], appears to yield quantitative predictions for several novel physical quantities, including the statistics of the blocking time ((2.4), (2.5), Fig. 2), and the distribution of the number of spin flips ((5.2), (5.3), Fig. 6).

Next, the present work demonstrates that the *a priori* uniform ensemble fails to describe the metastable states reached by Kawasaki dynamics. Systematic differences are indeed observed between numerical results and *a priori* predictions, especially in the pattern of spin correlations (Fig. 4) and in the distribution of domain sizes (Fig. 5). The latter are neither statistically independent nor exponentially distributed. These findings corroborate those of a previous work [8], devoted to constrained Glauber and Kawasaki dynamics, where we have already underlined qualitative differences between dynamical quantities and *a priori* predictions in the uniform ensemble.

To close up, we come back to the so-called 'Edwards hypothesis', as this concept has been quite commonly used in recent works. On the one hand, if this expression is taken in a broad sense, meaning that metastable configurations should be weighted with a uniform *a priori* measure, then it is invalidated in the one-dimensional kinetic Ising models investigated both in [8] and in the present work. On the other hand, the concept of flatness among metastable configurations had been put forward by Edwards in the rather specific context of granular materials subjected to 'gentle' dynamical perturbations. Accordingly, the Edwards hypothesis should rather be expected to apply to states reached under smoothly varying external conditions. The Edwards hypothesis '*stricto sensu*' has indeed been found to hold, at least as a good approximation, in a broad variety of granular systems and of spin models under tapping at a low intensity [21], and for some tapping mechanisms [15]. In this context, our findings do not invalidate the Edwards hypothesis '*stricto sensu*', as relaxational dynamics from a disordered initial state formally corresponds to tapping with an infinitely high intensity.

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