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The role of symmetry in the short-time critical dynamics

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Abstract

We analyse a method to determine the short-time exponent θ related to the critical initial slip in stochastic lattice models. In this method it suffices to start with an uncorrelated state with a vanishing order parameter instead of departing, as is usually done, from an initial state with a nonvanishing order parameter. The exponent θ is calculated by the time correlation of the order parameter. This method, deduced previously for up–down symmetry models, is extended here to include models with other symmetries. We also consider the extension to cover models with absorbing states.

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1. Introduction

The universal behaviour occurring in the first steps of a Monte Carlo simulation, the short-time dynamics, has been amply investigated [1–7] in the last few years. According to renormalization group arguments [1] the early-time behaviour of the order parameter (the magnetization, for example, in the case of the Ising model) follows a power law with a critical universal exponent θ. The numerical calculation of the exponent θ is performed by placing the system at the critical point and departing from a configuration where the order parameter m_0 is very small.

It has been shown [8], for systems with up–down symmetry, that it is possible to determine the exponent θ by starting with a configuration in which the order parameter is identically zero. In this approach one does not measure the order parameter, which is always zero, but its time correlation. If $M(t)$ denotes the instantaneous order parameter, the quantity

$$Q(t) = \langle M(t)M(0)\rangle \tag{1}$$

follows a power law

$$Q(t) \sim t^{\theta} \tag{2}$$

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where the initial configuration is uncorrelated and such that

$$\langle M(0)\rangle = 0. \tag{3}$$

The purpose of the current paper is to show that the procedure introduced in [8] for systems with up–down symmetry can be extended to systems with other symmetries. We show here that the results (1), (2) and (3) are general and can be applied to any lattice system described by a Markovian process such that the transition probability is invariant under a given group of symmetry operations. In particular, we apply the generalized scheme developed here to systems with antiferromagnetic ordering and to the Baxter–Wu model in a triangular lattice [9]. Employing this procedure it was recently calculated by numerical simulations [10], with an excellent precision, the exponent θ associated with the Baxter–Wu model with triplet interactions in a triangular lattice.

We consider also the short-time behaviour of intrinsic irreversible models with absorbing states, such as the contact process. In this case, we demonstrate here that it suffices to depart from a configuration with just one occupied site instead of starting from a configuration where the density of particles is finite and small. Therefore, the short-time behaviour of the order parameter is identical to the behaviour found by time-dependent simulations [11, 12] departing from a unique initial seed. In both methods it is necessary to place the system in its critical point.

2. Transition probability and symmetry

We consider the class of Markovian processes defined on a lattice whose probability distribution $P(\sigma, t)$ satisfies the equation

$$P(\sigma, t) = \sum_{\sigma'} T(\sigma, \sigma', t) P_0(\sigma') \tag{4}$$

where $T(\sigma, \sigma', t)$ is the probability of reaching the configuration σ from configuration σ' in an interval of time t and $P_0(\sigma')$ is the initial probability distribution. We use the notation $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ where N is the number of sites in the lattice and σ_i is the random variable attached to the ith site that takes two values.

If the system evolves in time according to a master equation (continuous time Markovian process)

$$\frac{\mathrm{d}}{\mathrm{d}t} P(\sigma, t) = \sum_{\sigma'} \{W(\sigma, \sigma') P(\sigma', t) - W(\sigma', \sigma) P(\sigma, t)\} \tag{5}$$

then the transition probability $T(\sigma, \sigma', t)$ are the elements of the matrix T given by

$$\widehat{T} = \exp\{t\widehat{W}\} \tag{6}$$

where $\widehat{W}$ is the matrix whose elements are

$$\widehat{W}(\sigma', \sigma) = W(\sigma', \sigma) \qquad \sigma' \neq \sigma \tag{7}$$

and

$$\widehat{W}(\sigma, \sigma) = -\sum_{\sigma'(\neq\sigma)} W(\sigma', \sigma). \tag{8}$$

Let R be a symmetry operation that leaves the transition probability invariant, or, equivalently, the matrix W invariant, that is

$$W(R\sigma, R\sigma') = W(\sigma, \sigma') \tag{9}$$

and by consequence

$$T(R\sigma, R\sigma', t) = T(\sigma, \sigma', t). \tag{10}$$

For simplicity, we will consider here only models in which the symmetry operation R changes the sign of the order parameter, that is,

$$M(R\sigma) = -M(\sigma) \tag{11}$$

and that $M(\sigma)$ is linear in σ, that is,

$$M(\sigma) = \sum_i \mu_i \sigma_i. \tag{12}$$

3. Time-dependent behaviour

We will focus on the time-dependent behaviour of the average

$$\langle M(\sigma)\rangle_t = \sum_\sigma M(\sigma) P(\sigma, t) \tag{13}$$

of the order parameter $M(\sigma)$. Its time evolution is given by

$$\langle M(\sigma)\rangle_t = \sum_\sigma \sum_{\sigma'} M(\sigma) T(\sigma, \sigma', t) P_0(\sigma') \tag{14}$$

where the initial state $P_0(\sigma)$ is uncorrelated with a nonzero magnetization. That is, the initial magnetization

$$\langle M(\sigma)\rangle_0 = \sum_\sigma M(\sigma) P_0(\sigma) = N m_0 \tag{15}$$

is nonzero, where N is the number of sites of the lattice and m_0 is a small quantity. As stated by the short-time scaling theory, the order parameter follows, at the critical point, a power-law behaviour

$$\langle M(\sigma)\rangle_t \sim m_0 t^\theta \tag{16}$$

for small values of m_0. According to this theory yet the initial state is prepared in such a way that all sites are uncorrelated with a nonzero (and small) initial order parameter m_0. In order to set up such an initial state, one attributes to each site a magnetization $m_i = m_0 \mu_i$. Or equivalentely, the spin of the ith site will be $\sigma_i = \mu_i$ with probability $(1 + m_0)/2$ and $\sigma_i = -\mu$ with probability $(1 - m_0)/2$. The initial probability $P_0(\sigma)$ can then be written as

$$P_0(\sigma) = \Phi_0 \prod_i \{1 + m_0 \mu_i \sigma_i\} \tag{17}$$

where

$$\Phi_0 = \frac{1}{2^N}. \tag{18}$$

Note that using equations (12) and (17) we can trivially find that

$$\langle M(\sigma)\rangle_0 = \sum_\sigma M(\sigma) P_0(\sigma) = N a m_0 \tag{19}$$

where a is the constant

$$a = \frac{1}{N} \sum_j [\mu_j]^2. \tag{20}$$

For small values of m_0, the expansion of the initial probability $P_0(\sigma)$ in powers of m_0 gives, up to linear terms in m_0, the following expression:

$$P_0(\sigma) = \Phi_0\{1 + m_0 M(\sigma)\}. \tag{21}$$

Substituting this expression in equation (14) we get

$$\langle M(\sigma)\rangle_t = \sum_{\sigma}\sum_{\sigma'} M(\sigma)T(\sigma,\sigma',t)\Phi_0 + \sum_{\sigma}\sum_{\sigma'} M(\sigma)T(\sigma,\sigma',t)\Phi_0 m_0 M(\sigma'). \tag{22}$$

Now, the first term on the right-hand side vanishes identically due to the following reasoning. Since the symmetry operation R leaves the transition probability invariant but changes the sign of the order parameter, we have

$$\sum_{\sigma}\sum_{\sigma'} M(R\sigma)T(R\sigma, R\sigma', t)\Phi_0 = -\sum_{\sigma}\sum_{\sigma'} M(\sigma)T(\sigma,\sigma',t)\Phi_0. \tag{23}$$

By a change of variable, $R\sigma \to \sigma$, the left-hand side of this equation equals the first term of the right-hand side of equation (22) so that it vanishes. Therefore

$$Q(t) = \lim_{m_0\to 0}\frac{\langle M(\sigma)\rangle_t}{m_0} = \sum_{\sigma}\sum_{\sigma'} M(\sigma)T(\sigma,\sigma',t)M(\sigma')\Phi_0 \tag{24}$$

and, from equation (16) it follows that

$$Q(t) \sim t^{\theta}. \tag{25}$$

4. Applications

4.1. Models with up-down symmetry

We begin with a simple example, namely the ferromagnetic Ising model coupled to a stochastic dynamics such as the Metropolis algorithm. The order parameter is defined by

$$M(\sigma) = \sum_i \sigma_i \tag{26}$$

where the summation is over all sites of the lattice. For the present case $\mu_i = +1$ for all sites of the lattice. Here the symmetry operation R, with the properties given by equations (10) and (11), is the one in which the up-down symmetry is observed, that is, the operation that changes the sign of each spin variable $\sigma_i \to -\sigma_i$.

The short-time behaviour for the Ising model has been already studied through the present formalism [8]. Besides, using this formalism, it has been possible to determine the short-time behaviour for several irreversible models (i.e., lacking detailed balance) [8, 13, 14] with up-down symmetry dynamics. These include for instance the majority vote model and similar nonequilibrium models [8, 15].

4.2. Models with antiferromagnet ordering

In this case the system is divided into two sublattices A and B. The order parameter is defined by

$$M(\sigma) = \sum_{i\in A}\sigma_i - \sum_{i\in B}\sigma_i. \tag{27}$$

Therefore, for this case one has $\mu_i = +1$ if $i \in A$ and $\mu_i = -1$ if $i \in B$. The symmetry operation R is a translation such that a given site of one sublattice goes into a site of the other sublattice. The short-time behaviour of a model with antiferromagnetic ordering was numerically studied by the present approach in [16].

4.3. Baxter–Wu model

We consider in this subsection the Baxter–Wu model with triplet interactions defined on a triangular lattice [9, 10]. The lattice is composed of three sublattices which we denote by A, B and C. The Baxter–Wu model does not have a global symmetry but semi-global symmetries. The Hamiltonian of the model and *a fortiori* the transition probability is invariant if we change the signs of two sublattices leaving the third invariant. It is convenient therefore to define three symmetry operations, denoted by R_A, R_B and R_C. The symmetry operation R_A changes the signs of the spins belonging to the sublattices B and C and leaves the signs of the spins of sublattice A invariant. Similar definitions can be stated for R_B and R_C. Each of these symmetry operations leaves the Baxter–Wu Hamiltonian invariant and *a fortiori* the transition probability invariant.

We take as the order parameter the magnetization of one of the sublattices, say, sublattice A, given by

$$M_A(\sigma) = \sum_{i \in A} \sigma_i. \tag{28}$$

Comparing it with equation (12) we have that $\mu_i = 1$ if $i \in A$ and $\mu_i = 0$ if $i \in B$ or $i \in C$. The symmetry operation R_B (or R_C) changes the sign of $M_A(\sigma)$ and leaves the transition probability invariant. According to the formalism developed in the previous section we conclude that

$$Q_A(t) = \lim_{m_0 \to 0} \frac{\langle M_A(\sigma) \rangle_t}{m_0} = \sum_{\sigma} \sum_{\sigma'} M_A(\sigma) T(\sigma, \sigma', t) M_A(\sigma') \Phi_0 \tag{29}$$

will behave as

$$Q_A(t) \sim t^{\theta}. \tag{30}$$

Equivalently, we may demonstrate that the analogous quantities $Q_B(t)$ and $Q_C(t)$ related to the magnetizations $M_B(\sigma)$ and $M_C(\sigma)$ of sublattices B and R_C, respectively, will behave as t^{θ}.

We may also use as the order parameter the total magnetization

$$M(\sigma) = \sum_{i} \sigma_i \tag{31}$$

which we write as the sum of the magnetizations of the three sublattices

$$M(\sigma) = M_A(\sigma) + M_B(\sigma) + M_C(\sigma) \tag{32}$$

which leads to

$$Q(t) = \sum_{\sigma} \sum_{\sigma'} M(\sigma) T(\sigma, \sigma', t) M(\sigma') \Phi_0. \tag{33}$$

Substituting (32) into (33) we see that $Q(t)$ is a sum of nine terms. The terms that involve magnetizations of distinct sublattices will vanish. For instance, the term that involves M_A and M_B will change sign by the use of the symetry operation R_A. The nonvanishing terms are the three terms that involve the same magnetization. One concludes that the quantity

$$Q(t) = Q_A(t) + Q_B(t) + Q_C(t) \tag{34}$$

and therefore will behave as t^{θ}. This procedure was used [10] to determine the exponent θ. The numerical results give very precise values for the exponent when compared with the results coming from simulations with nonzero initial magnetization.

5. Contact model

Now we discuss the short-time behaviour for models with an absorbing state. These models do not possess symmetry operations like the ones defined in the preceding sections. Due to this fundamental difference we need to proceed by introducing another approach. The simplest example of this type of model is the contact process [12]. Such model is defined in a lattice and each microscopic state is identified with $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ where $\sigma_i = 0$ or 1 according to whether the site i is empty or occupied by a particle. It evolves in time according to local Markovian rules where particles are catalitically created and spontaneously anihilated.

The initial probability is such that all sites are uncorrelated and the average $\langle \sigma_i \rangle = \rho_0$, that is,

$$P_0(\sigma) = \prod_i \{a(1-\sigma_i) + b\sigma_i\} \tag{35}$$

where

$$a = 1 - \rho_0 \qquad b = \rho_0 \tag{36}$$

is the total number of sites in the lattice.

Following the short-time scaling theory the order parameter $\langle n(\sigma) \rangle$ given by

$$\langle n(\sigma) \rangle_t = \sum_{\sigma'} \sum_{\sigma} n(\sigma) T(\sigma, \sigma', t) P_0(\sigma') \tag{37}$$

where

$$n(\sigma) = \sum_i \sigma_i \tag{38}$$

is the number of particle, behaves, at the critical point, as

$$\langle n(\sigma) \rangle \sim \rho_0 t^{\theta}. \tag{39}$$

Consequently, the quantity

$$Q(t) = \frac{1}{N} \lim_{\rho_0 \to 0} \frac{\langle n(\sigma) \rangle_t}{\rho_0} \tag{40}$$

has a similar behaviour in the early time regime

$$Q(t) \sim t^{\theta}. \tag{41}$$

For small values of ρ_0 we have

$$P_0(\sigma) = a^N \Phi_0(\sigma) + a^{N-1} b \sum_j \Phi_j(\sigma) \tag{42}$$

where

$$\Phi_0(\sigma) = \prod_i (1 - \sigma_i) \tag{43}$$

is the probability distribution such that the configuration $(0, 0, 0, \ldots, 0)$ (all sites empty) has probability 1 and the other configurations have zero probability,

$$\Phi_j(\sigma) = \sigma_j \prod_{i(\neq j)} (1 - \sigma_i) \tag{44}$$

is the probability distribution such that the configuration $(0, 0, \ldots, 1, \ldots 0)$ (a particle placed at the jth site and all other sites empty) has probability 1 and all other configurations have zero probability.

The average $\langle n(\sigma)\rangle_t$ can then be written as a sum of two parts

$$\langle n(\sigma)\rangle_t = a^N \sum_{\sigma'}\sum_{\sigma} n(\sigma)T(\sigma,\sigma',t)\Phi_0(\sigma') + a^{N-1}b\sum_{j}\sum_{\sigma'}\sum_{\sigma} n(\sigma)T(\sigma,\sigma',t)\Phi_j(\sigma'). \tag{45}$$

Since the contact process has an abosrbing state devoided of particles, the first term vanishes identically because $\Phi_0(\sigma)$ is the absorbing state. Therefore, using the translational invariance we obtain

$$Q(t) = \sum_{\sigma'}\sum_{\sigma} n(\sigma)T(\sigma,\sigma',t)\Phi_j(\sigma'). \tag{46}$$

To calculate numerically $Q(t)$, we start from a configuration with just one occupied site and determine the number of occupied sites at time t.

According to the scaling relations established for the time-dependent behaviour of the contact model in which the simulation is started with just one occupied site, the average number of particles $n_p(t)$ behaves as [11, 12]

$$n_p(t) \sim t^{\eta}. \tag{47}$$

As $Q(t)$ is identified with $n_p(t)$ so the exponent θ is identified with the exponent η [17].

Let us now calculate the time correlation of a given site, say the site j. It is given by

$$A(t) = \sum_{\sigma'}\sum_{\sigma} \sigma_j T(\sigma,\sigma',t)\sigma'_j P_0(\sigma') \tag{48}$$

and behaves, according to the short-time scaling theory, as

$$A(t) \sim t^{\lambda}. \tag{49}$$

Now

$$\sigma_j P_0(\sigma) = b\sigma_j \prod_{i(\neq j)} \{a(1-\sigma_i) + b\sigma_i\} \tag{50}$$

where we have used the obvious relations $\sigma_j(1-\sigma_j) = 0$ and $\sigma_j\sigma_j = \sigma_j$. Therefore, in the limit $\rho_0 \to 0$, we get

$$\lim_{\rho_0\to 0} \frac{1}{\rho_0}\sigma_j P_0(\sigma) = \Phi_j(\sigma). \tag{51}$$

Consequently,

$$B(t) = \lim_{\rho_0\to 0} \frac{A(t)}{\rho_0} = \sum_{\sigma'}\sum_{\sigma} \sigma_j T(\sigma,\sigma',t)\Phi_j(\sigma') \tag{52}$$

so that $B(t)$ behaves as

$$B(t) \sim t^{\lambda}. \tag{53}$$

Given that the initial particle seed is placed at a given site, the quantity $B(t)$ is the probability that this site be occupied at time t.

The exponent λ is related to dynamic exponent z by $\lambda = d/z - \theta$ [8]. Since the exponent θ was identified as the exponent η, it follows that $\lambda = d/z - \eta$. Now, from the hyperscaling relation for the contact process we have $d/z - \eta = 2\delta$ [12] where δ is the exponent associated with the survival probability. Therefore it follows that $\lambda = 2\delta$.

From the formalism developed here we conclude that the study of the short-time behaviour of the contact process, discussed in [17], is as a matter of fact equivalent to the study of this model by means of the time-dependent technique. Moreover, the critical exponents associated with the short-time dynamics for the contact model, as well as the relation among them, are equivalent to those found for the time-dependent simulations.

6. Conclusion

We have shown that the short-time critical exponent θ of several models invariant under a given group of symmetry can be calculated from the time correlation of the order parameter

$$Q(t) = \langle M(t)M(0)\rangle \tag{54}$$

where $\langle f(t)g(0)\rangle$ is a notation defined by

$$\langle f(t)g(0)\rangle = \sum_{\sigma}\sum_{\sigma'} f(\sigma)T(\sigma,\sigma',t)g(\sigma')\Phi_0. \tag{55}$$

This result follows from a generalization of the procedure introduced in [8]. We have also obtained similar formula for the contact process and shown that the short-time critical exponent θ is equal to time-dependent critical exponent η. Finally, the results obtained here for the continuous time Markovian processes can be straightforwardly extended to the probabilistic cellular automata (discrete time Markovian process).

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