Local Persistence and Blocking in the Two-Dimensional Blume–Capel Model

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Received on 26 March, 2004. Revised version received on 27 July, 2004

In this paper we study the local persistence of the two–dimensional Blume–Capel Model by extending the concept of Glauber dynamics. We verify that for any value of the ratio $\alpha = D/J$ between anisotropy D and exchange J the persistence shows a power law behavior. In particular for $\alpha < 0$ we find a persistence exponent $\theta_l = 0.2096(13)$, *i.e.* in the Ising universality class. For $\alpha > 0$ ($\alpha \neq 1$) we observe the occurrence of blocking.

Among the many relevant quantities of interest in the modelling of nonequilibrium dynamics of spin systems such as *first time passage* [1], which has been extensively discussed in the literature due to the appearance of non–trivial exponents in the power law behavior of the first return probability as function of time, another quantity of interest is that of *persistence*, *i.e.* the characterization of the time it takes for a particular spin *not* to change its state from its given $t = 0$ configuration. Defining $P(t)$ as the probability that a particular spin will not flip up to time t, at zero temperature temperature and for the Ising and Potts models this quantity was shown to behave as [2, 3]

$$P(t) \sim t^{-\theta_l}, \tag{1}$$

where the *persistence* exponent θ_l describes the nonequilibrium relaxation of the system. This has been determined through *coarsening* simulations since one expects that the fraction of spins which do not change up to t represents a good estimate of $P(t)$. As a consequence one may introduced a global version of the concept of persistence through the quantity $P_g(t)$ which represents the probability that the magnetization does not change its sign from its $t = 0$ value, as done in [4]. Recently one of the authors explored these ideas to determine the associated θ_g exponent in the Blume–Capel Model, in particular its behavior at the critical and tricritical points [8]. It was found that the exponent shows an abrupt change as one goes from the critical points ($\theta_g \simeq 0.23$, Ising universality class) to the tricritical one.

The purpose of this letter is to extend Glauber's dynamics to the Blume–Capel Model and to study the influence of the anisotropy on the exponent θ_l. For the sake of clarity, we start with a brief overview of the Ising model.

At $T = 0$ the dynamics can be greatly affected by local *blocking* configurations. Blocking is a phenomenon where a fraction of spins remains unchanged after t Monte-Carlo simulation steps. The energy necessary to overcome them might be so high as to render the system static. On the other hand, for $T \neq 0$ it becomes difficult to define domains because one might not be able to distinguish between true domains and spin flips due to thermal fluctuations. Nonetheless for the Ising Model these difficulties can be overcome and a power law decay for the fraction of persistent spins was found out in the whole low temperature phase [5]. The values found for the exponent were $\theta_l = 0.22, 0.22$ and 0.29 for $T = 0$, $T = T_c/3$ and $T = 2T_c/3$ respectively. Furthermore for $T > T_c$ an exponential cutoff was verified. Indeed, using a natural definition of persistence, the effects of blocking are sensitive to any temperature value, and power law happens only at $T = 0$. The dynamics is implemented as follows: define the excitation energy ΔE associated to the transition $\sigma_i \to -\sigma_i$ as $\Delta E = -2J\sigma_i S_i$, with S_i equal to the sum of nearest neighbors to σ_i. If $\Delta E < 0$ then the transition occurs with probability 1. For $\Delta E = 0$ it occurs with probability $1/2$ and the transition does not occur if $\Delta E > 0$.

All transition rules for $T = 0$ are derived from the Glauber dynamics function at $T > 0$, defined for 2-states models (i.e. $S = 1/2$) as:

$$w(\sigma_i \to -\sigma_i) = \frac{1}{2}\left[1 - \tanh\left(\frac{\Delta E}{2k_B T}\right)\right] \tag{2}$$

where k_B is the Boltzmann constant. We note that in the

limit $T \to 0$

$$w(\sigma_i \to -\sigma_i) \stackrel{T\to 0}{\to} \begin{cases} 1 & \text{if} \quad \Delta E < 0 \\ 1/2 & \text{if} \quad \Delta E = 0 \\ 0 & \text{if} \quad \Delta E > 0 \end{cases} .$$

One of most important questions in nonequibrium dynamics is however whether the $T > 0$ extension of the dynamics from the $T = 0$ case satisfies detailed balance:

$$w(\sigma_i \to -\sigma_i)/w(-\sigma_i \to \sigma_i) = \exp(-\frac{\Delta E}{k_B T}).$$

This condition is fulfilled by the Glauber dynamics of q–state spin models.

To extend these ideas to the Blume–Capel Model we start out with the Hamiltonian

$$H = -J \sum_i \sigma_i \sigma_{i+1} + D \sum_i \sigma_i^2 \tag{3}$$

where $\sigma_i \in \{-1, 0, 1\}$, $J > 0$ and D represents an anisotropy. As we shall see the behavior of the persistence exponent is strongly dependent on the value of $\alpha = D/J$ yielding a nontrivial extension of the Ising Model. To implement the Glauber dynamics in the ground state at ($T = 0$) we consider the excitation energy (in units of J) for the transition $\sigma_i \to \sigma_f$ as follows:

$$\Delta E/J = (\sigma_f - \sigma_i)\left[\alpha(\sigma_f + \sigma_i) - S_i\right] \tag{4}$$

with $S_i \in [-4, 4] \cap \mathbb{Z}$. To go from the $T = 0$ single spin Glauber dynamics of a 2–state system to a 3–state model is not straightforward and some rules have to be introduced. Let the energy differences in the transition from σ_i to any other two spin states σ_f^1 or σ_f^2 be represented by ΔE_1 and ΔE_2 respectively.

A simple dynamics that in the zero temperature limit of a Glauber dynamics satisfies detailed balance is the following: Choose between σ_f^1 and σ_f^2 with probability $1/2$, for example σ_f^1, then use the $T \to 0$ limit of (2) to accept or to reject the flip $\sigma_i \to \sigma_f^1$.

In our opinion however this is not the best choice, since it is biased in the sense that it does not make any distinction between situations as the following ones:

1. If $\Delta E_1 < 0$ and $\Delta E_2 < 0$, a the transition to the state with the smallest energy (the greater absolute energy gradient) will occur with probability 1, contrary to the rules of the simpler dynamics, where one chooses a state with probability $1/2$ and apply the $T = 0$ dynamics as defined;

2. If $\Delta E_1 = \Delta E_2 = 0$, the transition must occur to any state (σ_i, σ_f^1 or σ_f^2) with the same probability (1/3).

TABLE 1. Transition rules at T= 0 adoted for Blume–Capel Model

if $\Delta E_1 < 0$:	$\Delta E_1 < \Delta E_2$	:	$w(\sigma_i \to \sigma_f^1) = 1$
	$\Delta E_1 = \Delta E_2$	:	$w(\sigma_i \to \sigma_f^1) = \frac{1}{2}$
	$\Delta E_1 = \Delta E_2$	:	$w(\sigma_i \to \sigma_f^1) = 0$
if $\Delta E_1 = 0$:	$\Delta E_1 < \Delta E_2$	:	$w(\sigma_i \to \sigma_f^1) = \frac{1}{2}$
	$\Delta E_1 = \Delta E_2$	:	$w(\sigma_i \to \sigma_f^1) = \frac{1}{3}$
	$\Delta E_1 = \Delta E_2$	:	$w(\sigma_i \to \sigma_f^1) = 0$
if $\Delta E_1 > 0$:	$\{w(\sigma_i \to \sigma_f^1) = 0$		

Thus more convenient rules should be defined in order to establish probability transitions that mimic the Blume–Capel Model at $T = 0$. We propose the following rule

$$\begin{aligned} w(\sigma_i \to \sigma_f^1) &= \delta_{\xi(\Delta E_1),-1}\left(\tfrac{1}{2}\delta_{\Delta E_1,\Delta E_2} + \delta_{1,\xi(\Delta E_2 - \Delta E_1)}\right) \\ &+ \delta_{0,\xi(\Delta E_1)}\left(\tfrac{1}{3}\delta_{\Delta E_1,\Delta E_2} + \tfrac{1}{2}\delta_{1,\xi(\Delta E_2)}\right) \end{aligned} \tag{5}$$

where

$$\xi(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x = 0 \\ -1 & \text{if } x < 0 \end{cases}$$

and $\delta_{x,y}$ is Kronecker's delta function.

For the sake of clarity all transitions envisaged by this rule are given in the table 1.

Do these probabilities arise from a function that satisfies detailed balance for $T > 0$? Otherwise one may have the impression that our dynamics is somewhat arbitrary and that our results do not reflect a fundamental property of Blume–Capel Model.

For $T > 0$ we propose a dynamics we call Metropolis–Gibbs sampling approach[1]:

$$w(\sigma_i \to \sigma_f^{1,2}) = \frac{\exp(-\frac{\Delta E_{1,2}}{k_B T})}{1 + \exp(-\frac{\Delta E_{1,2}}{k_B T}) + \exp(-\frac{\Delta E_{2,1}}{k_B T})} \tag{6}$$

as a equivalent alternative to Glauber dynamics for the Blume–Capel Model at $T > 0$

In the limit $T \to 0$ all rules described in (table 1) can be obtained from this equation. Detailed balance is also guaranteed since

$$w(\sigma_i \to \sigma_f^1) = \frac{\exp(-\frac{\Delta E_1}{k_B T})}{1+\exp(-\frac{\Delta E_1}{k_B T})+\exp(-\frac{\Delta E_2}{k_B T})}$$

and

$$w(\sigma_f^1 \to \sigma_i) = \frac{\exp(\frac{\Delta E_1}{k_B T})}{1+\exp(\frac{\Delta E_1}{k_B T})+\exp(\frac{\Delta E_1 - \Delta E_2}{k_B T})},$$

[1] The name has its origin in two known dynamics, Metropolis and Heat Bath, this last also known as Gibbs Sampling. Our aproach mixes ideas from both.

once that

$$\frac{w(\sigma_i \to \sigma_f^1)}{w(\sigma_f^1 \to \sigma_i)} = \exp\left(-\frac{\Delta E_1}{k_B T}\right).$$

Finally with rules (table 1) Monte Carlo simulations were performed at $T = 0$ on a square lattice $L \times L$ ($L = 160$) to measure the fraction of spins that do not flip during t simulation steps. Since the sample number N_s does not play an important role due to the absence of significant statistical fluctuations (see *e.g.* [6]) we used $N_s = 200$ with 1000 MC steps. After some exploratory simulations a total of 60 different values of α within $\alpha \in [-3, 3]$ where chosen.

After the 300th MC step convergence to power laws are found, as can be seen in Fig. 1. For $\alpha < 0$ we obtained the exponent $\theta_l = 0.214(3)$ by measuring directly the slope in the interval $[300, 1000]$, with error bars obtained using 5 different bins. A more precise estimate can be obtained using the definition of the effective exponent (local slope):

$$\theta_l(t) = \frac{1}{\ln r} \ln \frac{P_l(t)}{P_l(t/r)} \tag{7}$$

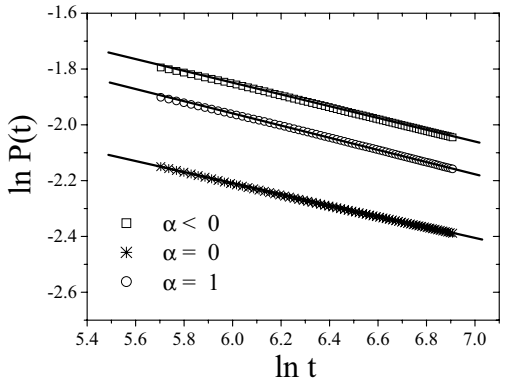

Figure 1. The numerical estimate of the probability $P(t)$ in (1) as described in the text.

For $r = 10$ and $t = 1000$ we obtain $\theta_l = 0.2096(13)$. The same power law behavior was observed for $\alpha = 0$ and $\alpha = 1$, however with slightly different exponents, as can be seen in table 2.

TABLE 2. Local persistence exponent values of Blume–Capel Model.

	$\alpha < 0$	$\alpha = 0$	$\alpha = 1$
θ_l	0.2096(13)	0.1964(34)	0.1993(21)

For positive values of α ($\neq 1$) the system shows blocking, i.e., the fraction of spins that remain no changed after t Monte Carlo steps, as can seen in Fig. 2. However a distinction must be made: in $\alpha \in]0, 1[$ the persistence has a fast decay and reaches a constant value $P(t \to \infty) \simeq 0.322$, while for $\alpha \in]1, 2]$ the value is $P(t \to \infty) \simeq 0.246$. For $\alpha = 2$, $P(t \to \infty) \simeq 0.287$) and when $\alpha > 2$ there is full blocking with $P(t \to \infty)$ frozen to the value $\simeq 0.333$ (initial mean fraction of spins is null). In $d = 2$ and $T = 0$ this is due to the fact that for $\alpha > 2$ the predominant phase is a configuration with all spins zero.

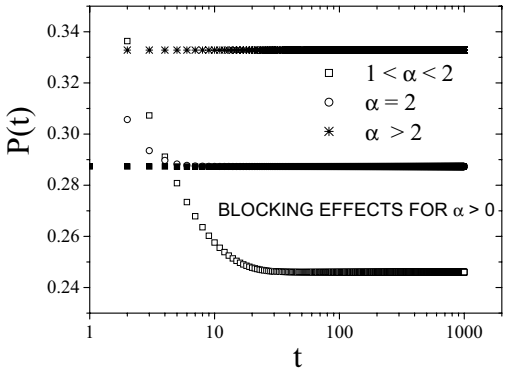

Figure 2. Blocking effects for positive values of $\alpha(\neq 1)$.

Our values for $\alpha < 0$ are in agreement with more recent results for the Ising Model, namely [7]

$$\theta_l = 0.209(2) \tag{8}$$

The point $\alpha = 0$ separates two distinct regions: a power law behavior for negative values of α and a blocking phase for positive values of this ratio. At $\alpha = 0$ we have a power law behavior but with a different exponent.

Another interesting behavior is observed for $\alpha = 1$, where a robust power law separates two different blocking "phases". The point $\alpha = 2$ also divides two regions of distinct blocking behavior: the $1 < \alpha < 2$ region and the full–blocking region $\alpha > 2$.

To conclude, our results show that a nontrivial behavior in stochastic persistence can appear as one extends the Ising Model to allow for higher "spins" and anisotropy effects as measured by our parameter α. In particular for $\alpha < 0$ one has a pure 2–state Ising behavior; the same is not observed for different values of α, as discussed in the text. It would be interesting to test these ideas in other stochastic systems in order to see whether some sort of nontrivial behavior might be found.

Acknowledgements

R.S. dedicates this paper to the memory of his brother Ricardo D. da Silva. S.R.D. would like to thank the Mathematical Physics Group at the University of Queensland for their hospitality.

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