

Diffusive thermal dynamics for the spin- S Ising ferromagnet

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Abstract. We introduce an alternative thermal diffusive dynamics for the spin- S Ising ferromagnet realized by means of a random walker. The latter hops across the sites of the lattice and flips the relevant spins according to a probability depending on both the local magnetic arrangement and the temperature. The random walker, intended to model a diffusing excitation, interacts with the lattice so that it is biased towards those sites where it can achieve an energy gain. In order to adapt our algorithm to systems made up of arbitrary spins, some non trivial generalizations are implied. In particular, we will apply the new dynamics to two-dimensional spin-1/2 and spin-1 systems analyzing their relaxation and critical behavior. Some interesting differences with respect to canonical results are found; moreover, by comparing the outcomes from the examined cases, we will point out their main features, possibly extending the results to spin- S systems.

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1 Introduction

The Ising model has been extensively studied both by analytical and computational methods; the latter are especially useful for complex and high dimensional lattices and rely, for example, on Monte Carlo methods [1]. This implies to find a prescription for updating the spin system and an algorithm which determines if the suggested spin-flip can be accepted.

The first procedure is the most subtle and it is usually chosen so that it can be easily implemented (it typically consists in a sweep along parallel lattice lines) while the latter often refers to well-known algorithms such as the Glauber one.

Here our aim is not to find an efficient algorithm, but rather to realize a thermal dynamics physically consistent, which possibly violates the detailed balance condition. In particular, we refer to [2] where a diffusive dynamics was introduced: the spin flips are induced by a random walker hopping across the sites of the lattice. This model was inspired by some non-stoichiometrical compounds [3] where diffusing excitations (for example charged carriers) affect the spin dynamics. Then, in our dynamics, the walker is meant as a local excitation diffusing throughout the whole sample and interacting with the magnetic arrangement. Moreover, we suppose the walker to be biased towards

those sites where a spin-flip is energetically more favorable. This technique is not only more natural than the traditional ones, but it can also be applied to irregular lattices represented by graphs.

The previous work succeeded in defining a new, well-working dynamics, nevertheless the algorithm introduced was expressly meant for a spin-1/2 system. Its extension to the general spin- S case is non trivial since, while in the spin-1/2 case each spin of the lattice allows only one possible new state, here the spin status is not binary and a manifold choice occurs. Therefore, a further random process has to be introduced: apart from the one concerning the selection of the nearest-neighbor to move towards, we also have to take into account the one relevant to the variety of states accessible to the spin considered. Then, in this work, we developed a new algorithm able to be applied to systems made up of discrete spins with an arbitrary number of states. Not only, we also wondered to what extent results found in [2] depend on the special algorithm and spin model taken into account. In order to do so we implemented our dynamics on both spin-1/2 (as a test) and spin-1 (as first example) systems.

The remaining of the paper is organized as follows. In Sections 2 and 3 we explain the model and the new algorithm, Sections 4 and 5 are devoted to the analysis of the results: thermodynamics of the system and relaxation at low temperature, respectively. Finally, in Section 6 we discuss our outcomes.

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2 The model

The most general spin-1 Ising model with up-down symmetry is the BEG model [4], whose Hamiltonian reads:

$$\mathcal{H} = -J \sum_{j \sim i}^N \sigma_i \sigma_j - D \sum_{j \sim i}^N \sigma_i^2 \sigma_j^2 - K \sum_i^N \sigma_i^2, \quad (1)$$

where the first two sums are over all nearest-neighbor pairs on the lattice, the last is over all sites and $\sigma_i = \pm 1, 0$. This model was originally introduced to study phase separation and superfluidity in ^3He - ^4He mixtures; then it has been applied to describe properties of multicomponent fluids, microemulsions, superconductor alloys and electronic conduction models [5–7]. Here we consider the particular situation with $K = D = 0$ and $J \neq 0$ in order to preserve the analogy with the spin-1/2 case and to concentrate on the dynamical aspects.

The analysis of the diffusive dynamics is carried out from the numerical point of view adopting a two dimensional array of spins, so that, as mentioned above, results obtained for the spin-1/2 are useful as a test by comparison with those analytically known and relevant to the canonical equilibrium state. Unfortunately, this is not possible for the spin-1 case as there exists no exact solution, hence we will refer to earlier works mainly dealing with Monte Carlo simulations, finite-size scaling, high- and low-temperature expansions [8–13].

However, just a relatively small number of works about critical exponents for the $S \geq 1$ Ising model has been published. Those works are mostly numerical and they confirm the exponents independence on the spin magnitude, as consistent with the renormalization group theory [14]. Therefore, our work, though based on a non-traditional dynamics, would offer an insight into this matter. In fact, also encouraged by the interesting outcomes found in [2], we mainly focused on the critical aspects.

3 Diffusive thermal dynamics

We refer to the algorithm introduced in [2] and we improve it so that it can be easily adapted to systems made up of spins with an arbitrary number of states q . In fact, as already mentioned, that kind of algorithm is an exclusive for systems made up of binary valued spins.

The relaxation dynamics is realized by a random walker diffusing through the sites of the Ising lattice. In general, the walker on a site i has $(2d + 1)q$ possibilities: it can move towards one of its $2d$ nearest neighbors j or stop and it can flip the spin relevant to the reached site or leave it unchanged.

More precisely, the walker moves from i to j realizing the magnetic configuration \mathbf{s} according to the normalized probability:

$$\mathcal{P}_T(\mathbf{s}, i, j) = \frac{p_T(\mathbf{s}, j)}{\sum_{\{\mathbf{s}'\}} \sum_{j=0}^{2d} p_T(\mathbf{s}', j)}. \quad (2)$$

In this equation $\{\mathbf{s}'\}$ is the whole of magnetic configurations which can be realized from the current one and

$$p_T(\mathbf{s}, k) = \frac{1}{1 + e^{[\beta \Delta E_k(\mathbf{s})]}} \quad (3)$$

represents the probability of spin-flip relevant to the site k , being

$$\Delta E_k(\mathbf{s}) = (\sigma_k - \sigma'_k) \sum_{j \sim i} \sigma_i, \quad (4)$$

the energy variation consequent to the process. Equation (3) has been derived from the usual Glauber probability [15]:

$$P_T^G(\mathbf{s}, k) = \frac{e^{-\beta E_n}}{\sum_{m=1}^q e^{-\beta E_m}} \quad (5)$$

which represents the probability that the selected spin k has the value $\sigma_k = n$, being E_n the energy relevant to that configuration. Note that the previous expression can be rewritten as

$$P_T^G(\mathbf{s}, k) = \frac{1}{1 + \sum_{\substack{m=1 \\ m \neq n}}^q e^{\beta \Delta E_m}} \quad (6)$$

with $\Delta E_m = E_n - E_m$ and it reduces to equation (3) when $q = 2$. However, we adopt equation (3) in each case because it is more direct and it also reveals to be more efficient.

You can notice that the magnetic configuration of the system, as well as the position of the walker, can remain unchanged and that the diffusion of the walker is biased towards those sites where it can achieve a gain in the energy.

There are some important consequences of the fact that such a dynamics includes both the walker motion on the lattice and the magnetic evolution of the lattice itself. In particular, the analytical approach is made rather difficult and the detailed balance is explicitly violated. In fact, the latter imposes the quite restrictive condition:

$$p_\nu P(\nu \rightarrow \mu) = p_\mu P(\mu \rightarrow \nu), \quad (7)$$

according to which the overall rate at which transitions from one state ν to another state μ happen is the same for the reverse process. However, in our system, the probability of being in a state ν , as well as the probability of making a transition $\nu \rightarrow \mu$, are non trivial functions of both the magnetic arrangement and the position of the walker on the lattice, which involves that equation (7) does not hold. In order to clarify this subtle point, a further insight is provided. Suppose the transition $\mu \rightarrow \nu$ represents the walker jumping from site i to j , realizing the spin-flip $\sigma_j \rightarrow \sigma_j^*$. The reverse transition is obviously impossible, since it requires the walker to flip the spin relevant to the starting site, $\sigma_j^* \rightarrow \sigma_j$, while jumping from j to i . As mentioned at the beginning of this section, this kind of flip is forbidden by our dynamics so that $P(\nu \rightarrow \mu) = 0$.

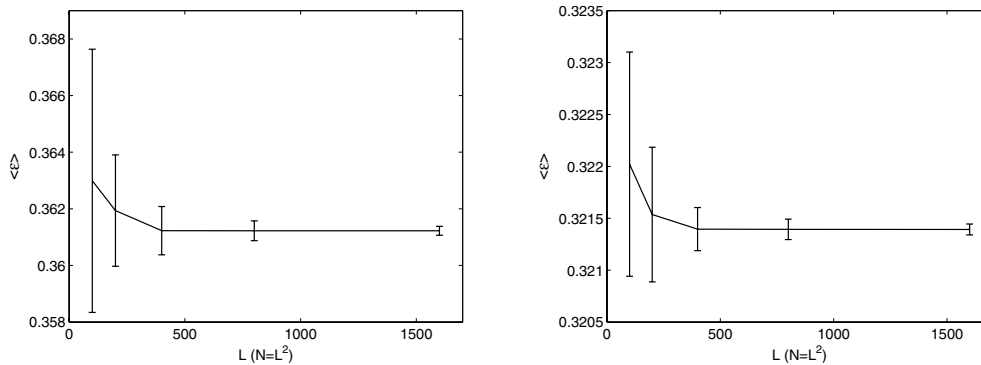


Fig. 1. Finite size scaling for the specific energy of a spin-1/2 (left panel) and spin-1 (right panel) Ising system subject to the diffusive dynamics described in Section 3 at $T = 2.40$ and $T = 1.56$ respectively. All the measurements were carried out in the stationary regime and the error bars represent the fluctuations about the average values.

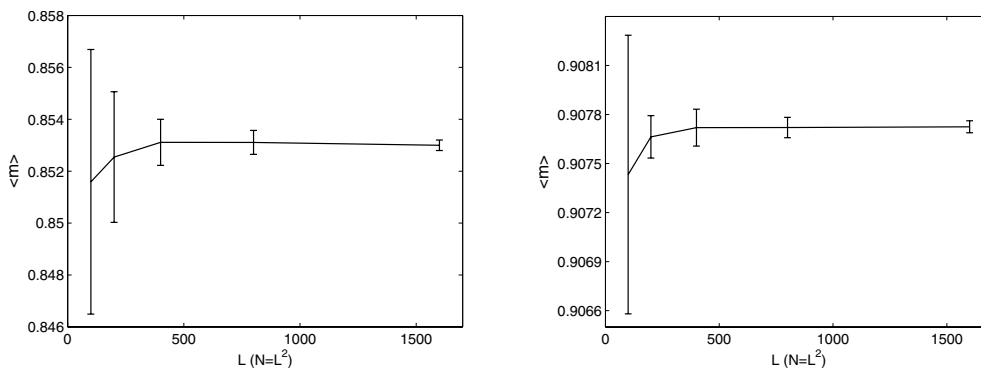


Fig. 2. Finite size scaling for the specific magnetization of a spin-1/2 (left panel) and spin-1 (right panel) Ising system subject to the diffusive dynamics described in Section 3 at $T = 2.40$ and $T = 1.56$ respectively. All the measurements were carried out in the stationary regime and the error bars represent the fluctuations about the average values.

On the other hand, since the walker can reach any lattice site, whatever the magnetic arrangement, both p_μ and p_ν are strictly positive quantities; as a result equation (7) is false.

Note that the violation of the detailed balance is consistent with our dynamics intent: it is not meant to recover the canonical distribution, but rather to model some possible physical processes making the spin system evolve.

Analogous considerations can be drawn for other kinds of diffusive dynamics employing random walkers.

On the other hand, a fundamental difference with the algorithm suggested in [2] is that here, once the new site selected, the corresponding probability is not determined because we have also to specify the magnetic configuration \mathbf{s} candidate to be realized. Of course, in the spin-1/2 case this is not necessary because, once the new site chosen, there is just one new magnetic configuration which can be considered.

Thus, our algorithm generalizes the previous one: now it includes all kinds of new scenarios so that it can properly work also for $S > 1/2$ cases.

Our analysis will be performed mainly by means of numerical simulations keeping fixed the value of the exchange interaction constant ($J = 1$) and setting periodic boundary conditions for the square lattice where spins are placed on. In fact, it is clear that an equilibrium situation can be reached only after the random walker realizing the

dynamics has visited every sites of the system a sufficient number of times; this in particular selects the periodic boundary conditions as the most natural for the problem. Moreover, we deal with just one walker postponing the case of a larger density to next works.

4 Thermodynamic of spin-1/2 and spin-1 systems

In this section we describe the results pertaining to spin-1/2 showing their consistency with those in [2] and then we will move to spin-1 delaying a global discussion to Section 6.

In both cases the dynamics realized by the random walker actually drives the system to a thermodynamically well-behaved steady state, highly independent on the initial conditions. As we will see later, results relevant to the critical exponents will provide another strong signature that the stationary state reached by the system is actually an equilibrium state, though it is non trivially different from the canonical equilibrium of the Ising model. In fact, we verified that also for our diffusive dynamics the normalized joint probability $\tilde{\mathcal{P}}(\epsilon, m, T)$, introduced in [2], depends on T .

In Figures 1 and 2 the average values of the specific energy and magnetization are plotted for systems with different sizes, at a fixed value of the temperature parameter.

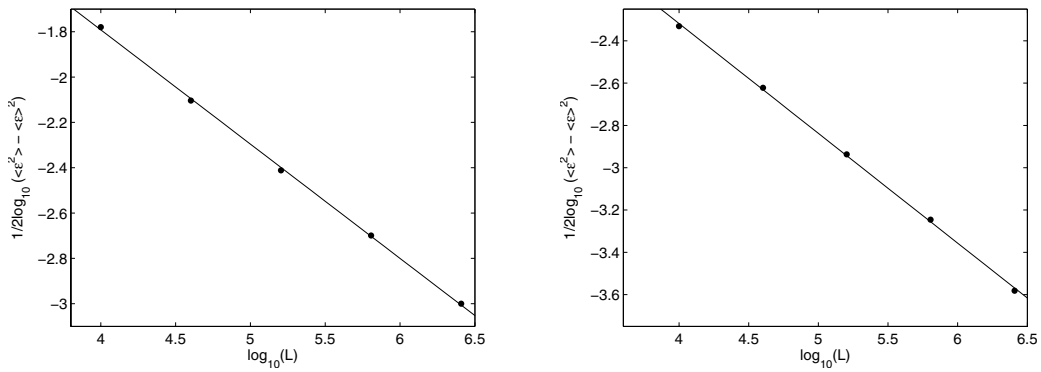


Fig. 3. Finite size scaling for the fluctuation about the average value of the specific energy for a spin-1/2 (left panel) and spin-1 (right panel) Ising system subject to the diffusive dynamics described in Section 3 at $T = 2.40$ and $T = 1.56$ respectively. The slopes of the linear fit (line) of the measured data (\bullet) -0.50 ± 0.01 and -0.51 ± 0.02 are in good agreement with the expected value -0.5 . All the measurements were carried out in the stationary regime.

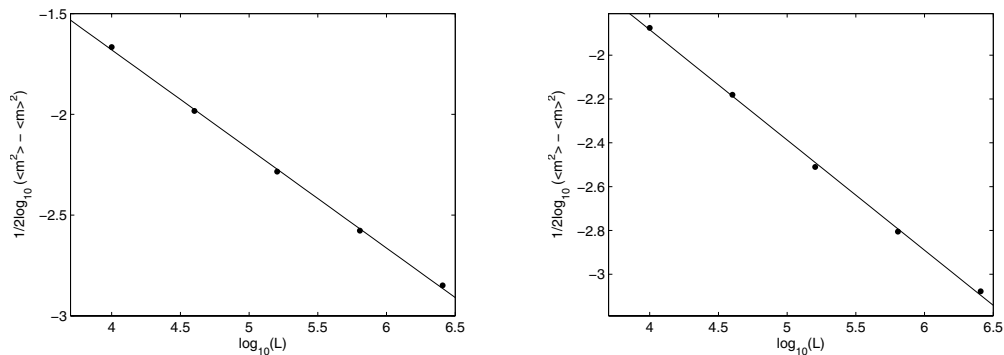


Fig. 4. Finite size scaling for the fluctuation about the average value of the specific magnetization for a spin-1/2 (left panel) and spin-1 (right panel) Ising system subject to the diffusive dynamics described in Section 3 at $T = 2.40$ and $T = 1.56$ respectively. The slopes of the linear fit (line) of the measured data (\bullet) -0.49 ± 0.02 and -0.50 ± 0.02 are in good agreement with the expected value -0.5 . All the measurements were carried out in the stationary regime.

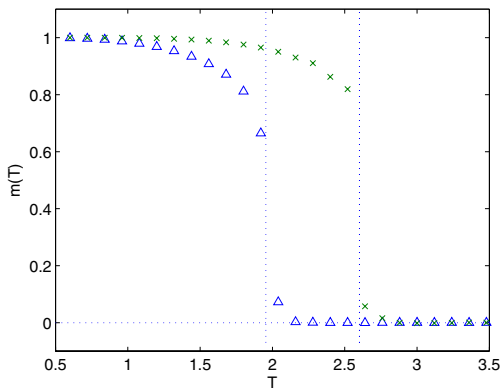


Fig. 5. Specific magnetization for a 400×400 spin-1/2 (\times) and spin-1 (\triangle) Ising system. The vertical dashed lines are placed at the critical values of the temperature.

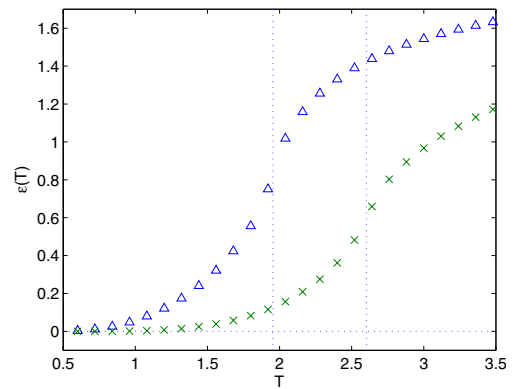


Fig. 6. Specific energy for a 400×400 spin-1/2 (\times) and spin-1 (\triangle) Ising system. The vertical dashed lines are placed at the critical values of the temperature.

Figures 3 and 4 show the expected scaling behavior for the fluctuations about the average value of the specific thermodynamic observables which decrease as the inverse square root of the lattice size. Now let us consider Figures 5 and 6: the average values of magnetization and energy are plotted versus temperature. For spin-1/2 a phase transition is apparent at about $T = 2.6$ which is a value significantly higher than the exact critical temperature

(we will deeply return on this feature later). For spin-1 we see similar, but somehow left-shifted, curves which clearly suggest $T_c^{S=1} < T_c^{S=1/2}$. Analogous considerations can be made from Figure 7 where relevant magnetic susceptibility and specific heat are depicted: their profiles are consistent with the theory and highlight that a phase transition happens at a well defined temperature.

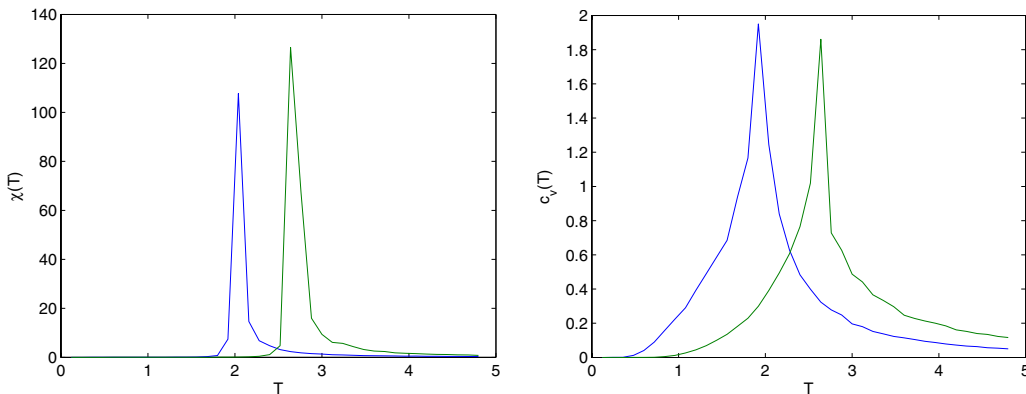


Fig. 7. Magnetic susceptibility (left panel) and specific heat (right panel) for a 400×400 Ising system of spin-1/2 and spin-1. The two cases are easily distinguishable since the former displays a higher critical temperature.

Note that these results do not depend on the particular initial configuration which can, at least, affect the orientation of the asymptotic arrangement. The evolution of the system when the initial magnetization is very low is quite interesting, especially in the spin-1 case, and it will be treated in the next section. Now we focus our attention on the critical behavior of the systems, i.e. the properties featured nearby the phase transition. From general theoretical considerations, based on the renormalization group theory, we expect that the critical exponents do not depend on the spin magnitude, but they are characterized by the dimensionality of the system and by its order parameter [14]. Nevertheless, it is not trivial that a diffusive dynamics, generating a non canonical ensemble, does not affect the universality class.

First of all, we observe that, like for the canonical Ising model, the phase transition induced by the diffusive dynamics exhibits a singular behavior for the thermodynamic functions. In this context it is important to stress that specific heat and magnetic susceptibility were calculated as fluctuations according to other studies of Ising system where fluctuation-dissipation theorem does not strictly apply.

In Figure 8 we plotted the data of magnetization fitted by the power law

$$m(T) \sim |T - T_c|^\beta. \quad (8)$$

These data were used to estimate both the transition critical temperature and the relevant critical exponent. The estimated values are respectively $T_c^{S=1/2} = 2.602 \pm 0.001$ and $\beta = 0.123 \pm 0.005$. The latter is in good agreement with the relevant critical exponent of the two-dimensional Ising model, while the former is significantly higher than the exact one $T_c^{Ising} = \frac{2J}{\log(1+\sqrt{2})} \approx 2.269$, but there is a fairly good agreement with the value $T_c^{S=1/2} = 2.612 \pm 0.001$ found in [2]. As shown in Figure 9 specific heat behaves like the function

$$f(T) = a + b \log(|T - T_c|) \quad (9)$$

which corresponds to a logarithmic divergence for the observable at the critical temperature. In Figure 10 we

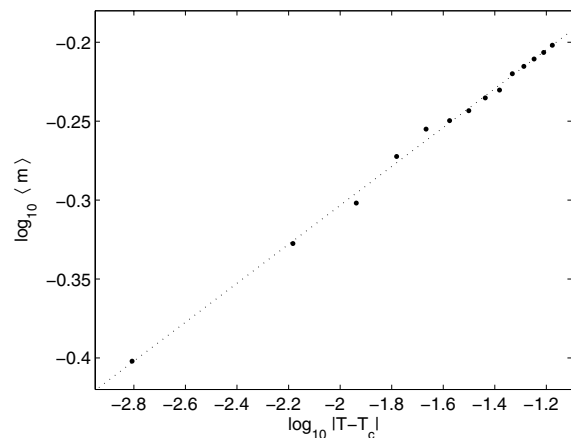


Fig. 8. Log-log scale plot of magnetization versus $|T - T_c|$ for a spin-1/2 Ising system subject to the diffusive dynamics (\bullet). The measures were performed on a 1600×1600 array of spins. The dotted line is the best fit: $y = A|T - T_c|^\beta$. The estimated values for the critical temperature and for the exponent are $T_c = 2.602 \pm 0.001$ and $\beta = 0.123 \pm 0.005$, respectively. The latter is consistent with the relevant canonical one.

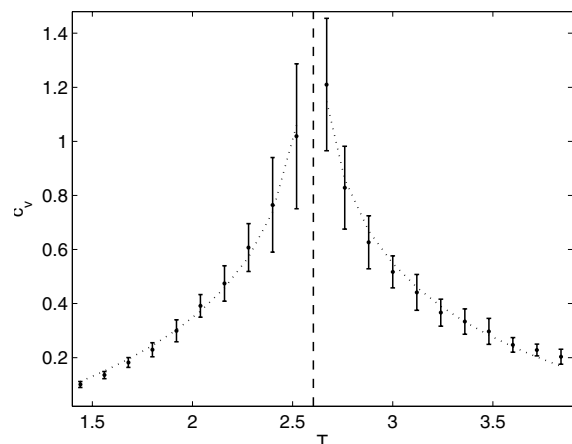


Fig. 9. Specific heat for a spin-1/2 Ising system subject to the diffusive dynamics (\bullet). The dotted curves fitting the data are of the form $f(T) = a + b \log(|T - T_c|)$. The vertical dashed line indicates the estimated value of the critical temperature.

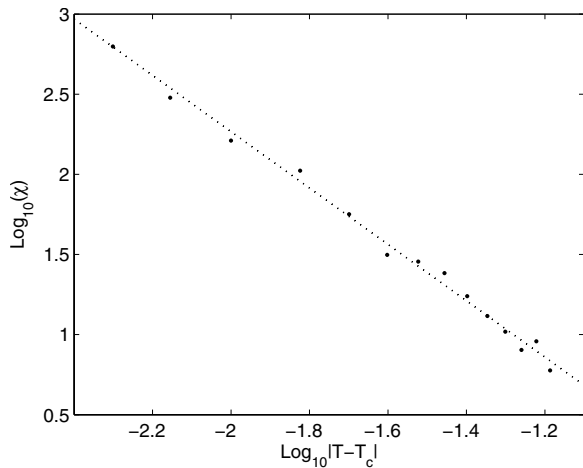


Fig. 10. Log-log scale plot of magnetic susceptibility versus $|T - T_c|$ for a spin-1/2 system subject to the diffusive dynamics (\bullet). The straight line fitting the data has a slope $\gamma = 1.761 \pm 0.049$ consistent with the canonical critical exponent.

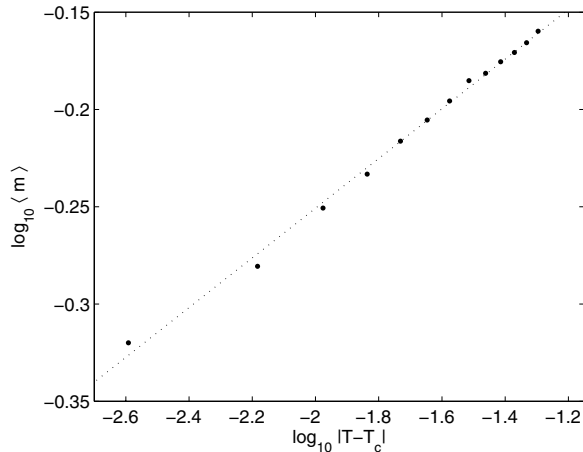


Fig. 11. Log-log scale plot of magnetization versus $|T - T_c|$ for a spin-1 Ising system subject to the diffusive dynamics (\bullet). The measures were performed on a 1600×1600 array of spins. The best fit is represented by the dotted line $y = A |T - T_c|^\beta$. The estimated values for the critical temperature and for the exponent are $T_c = 1.955 \pm 0.002$ and $\beta = 0.126 \pm 0.005$, respectively; the latter is consistent with the relevant canonical one.

represented a log-log scale plot of magnetic susceptibility which is suitably fitted by a straight line with slope $\gamma = 1.761 \pm 0.049$. This means that

$$\chi(T) \sim |T - T_c|^\gamma. \quad (10)$$

Hence, for the three critical exponents measured, there is a very good agreement with the canonical case: $\beta^{Ising} = 1/8$, $\alpha^{Ising} = 0$ and $\gamma^{Ising} = 7/4$.

Now let us consider the spin-1 system: analogous results have been gathered. Figure 11 shows that magnetization data are consistent with the same power law of equation (8) with critical exponent $\beta = 0.126 \pm 0.005$ and critical temperature $T_c = 1.955 \pm 0.002$ higher than values

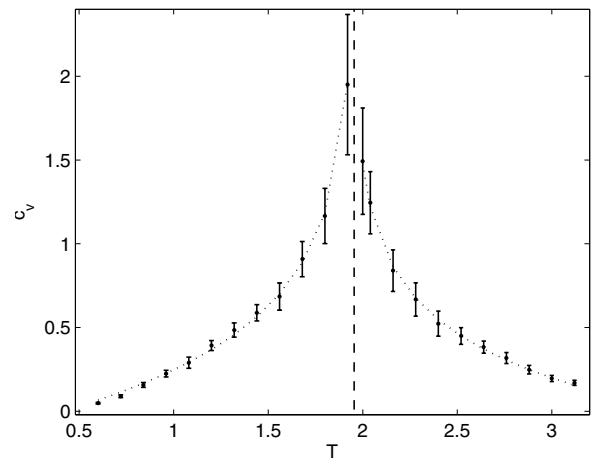


Fig. 12. Specific heat for a spin-1 Ising system subject to the diffusive dynamics (\bullet). The dotted curves fitting the data are of the form $f(T) = a + b \log(|T - T_c|)$. The vertical dashed line indicates the estimated value of the critical temperature.

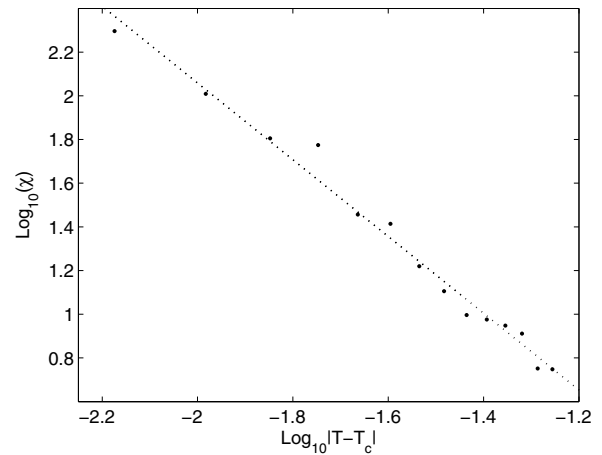


Fig. 13. Log-log scale plot of magnetic susceptibility versus $|T - T_c|$ for a spin-1 system subject to the diffusive dynamics (\bullet). The straight line fitting the data has a slope $\gamma = 1.756 \pm 0.064$ consistent with the canonical critical exponent.

($T_c^{S=1} \approx 1.695$) obtained in [8–12]. Also the specific heat behaves according to equation (9) hence, again, a logarithmic divergence is obtained at about T_c (Fig. 12). Finally, the magnetic susceptibility follows the same power law of equation (10) with $\gamma = 1.756 \pm 0.064$ (Fig. 13). Results explained so far point out that, different models are similarly affected by the diffusive dynamics. In particular, the analyzed spin-1/2 and spin-1 Ising systems subject to our dynamics share the same universality class (which is consistent to analytical results), despite their critical temperatures are both 15% circa larger than their canonical counterparts.

As observed in [2], such a quantitative difference cannot be overcome by a simple rescaling of the temperature; conversely, the exact critical temperature was restored by increasing the density of walkers.

5 Relaxation

In this section we deal with the properties featured by the system when its initial configuration is paramagnetic and the temperature is low ($T \ll T_c$). Of course, the time required by the walker to lead the system to equilibrium is much larger than that needed when the system is initialized ferromagnetic.

For both spin-1/2 and spin-1 systems, starting with a low magnetization (whatever their arrangement), we notice the formation of domains characterized by a different orientation of their spins. Carrying on with the simulation, one of the domains can prevail against the others and a nearly ferromagnetic situation is established. However, at very low temperatures, this evolution may be delayed by the appearance of metastable states. These states correspond to regularly shaped domains so that the lattice appears striped. Such configurations also occur when a non-diffusive dynamics is adopted, though less often. We also compared the typical magnetic configurations pertaining to our diffusive dynamics to the more traditional Metropolis dynamics, exploiting the typewriter sequence updating. Interestingly, in the former case, clusters display smoother boundaries, especially for the spin-1/2 system (Figs. 14, 15). A deep study of the geometry of these clusters will be the subject of a future paper [16].

Now it is worth deepening the particular role played by the null spin in the case $S = 1$. The state $\sigma = 0$ provides not only a further option for the spin variables, but it also shows the property of being energetically neutral. As a consequence, null spins are not expected to form wide clusters, but rather to be found on the boundaries between positive and negative clusters. In particular, they are likely to stay on those sites such that $\sum_{j=1}^4 \sigma_j = 0$.

Finally, we note that, in the spin-1 system, the existence of a third state makes transitions among spin states more likely to happen. In fact, in general, when the number of states increases, there is also a rise in the number of possible convenient events so that a spin-flip gets more and more probable. This consideration also provides a reason why the critical temperature for a spin-1 system must be lower than its spin-1/2 counterpart. An analogous consideration may also be applied to spin- S arrangements with $S > 1$ [17].

6 Conclusions

The new algorithm we introduced realizes, by means of a random walker, a diffusive dynamics to be applied to an Ising ferromagnet. Such a model provides a proper alternative to the usual methods of updating the spin-system and it can also be useful in order to investigate the interaction of diffusing excitations with spins.

A fundamental feature of our algorithm is that it can be adapted to a number of other physical systems, as it simply requires the system to be represented by an arbitrary arrangement of sites, each one related to a discrete variable, and to be endowed with a proper set of local dynamics rules. Due to the arbitrariness of the arrangement, we can consider systems implemented on general

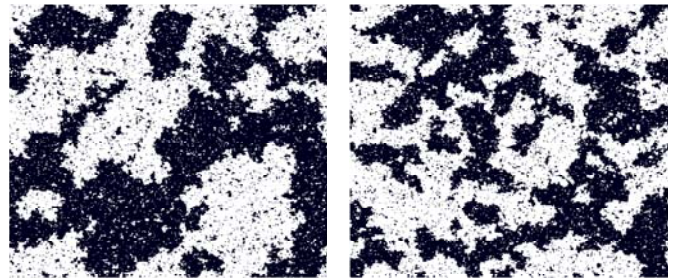


Fig. 14. Two snapshots showing typical magnetic configurations for a 400×400 spin-1/2 Ising lattice with $\langle m \rangle = 0.82$ subject to the diffusive dynamics at $T = 2.46$ (left panel) and to the Glauber one at $T = 2.15$ (right panel). Note that the left figure shows smoother boundaries and that the same magnetization is attained for different temperatures.

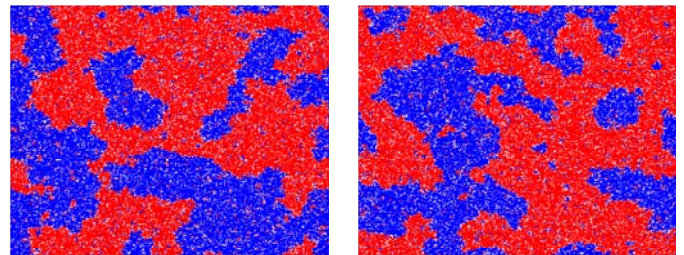


Fig. 15. (Color on line) Two snapshots showing typical magnetic configurations for a 400×400 spin-1 Ising lattice with $\langle m \rangle = 0.78$ subject to the diffusive dynamics at $T = 1.84$ (left panel) and to the Glauber one at $T = 1.60$ (right panel). Null spins are colored white. Notice that the difference between these pictures is not so marked as that found in the previous figure.

discrete networks, ranging from completely disordered to fractal. Moreover, as a result of our extension (see Sect. 3), the walker realizing the dynamics can deal with finite-multistate local variables. Therefore, our algorithm can also be applied to the q -state Potts model and, clearly, to all the physical systems related to that model (such as lattice gas, site and bond percolation, discrete vertex model). Finally, as far the local dynamics rules, the equations described in Section 3, could be properly modified according to the particular Hamiltonian pertaining to the system taken into account. For example, for the Randomly Coupled Ferromagnet [18], a different estimate of the energy variation consequent to a spin-flip would be reflected by the probability of equation (2).

However, notice that, in general, the peculiar diffusive character of the dynamics is preserved.

As far the thermodynamic of the spin systems considered in this work, we found that the diffusive character of the dynamics leads to a critical temperature which is significantly larger than the canonical one, notwithstanding the universality class is preserved. This result constitutes an interesting confirmation that, according to the renormalization group theory, the universality class is just concerned with the geometry of the lattice and the symmetry of the ordered state. In fact, as supported by our simulations, the critical exponents we measured are the same for spin-1/2 and spin-1 Ising systems (on a squared lattice),

and, even more interestingly, they are also unaffected by our non-canonical dynamics. Moreover, the rise in the critical temperature and the conservation of the universality class are very effects of the diffusive dynamics as they seem not to be due to a particular choice of the model.

The preservation of the universality class also suggests that the stationary state reached by the system has to be regarded as a non-canonical equilibrium state. In addition, we recall that such a steady state is definitely independent on the initial conditions. On the other hand, by increasing the density of the walkers, we expect to recover the canonical Boltzmann distribution (as shown in [2]).

Of course, it would be quite interesting also to study what happens on spin- S ($S > 1$) systems or on higher dimensional lattices.

However, what seems to be more interesting up to now is a geometrical analysis of magnetic clusters and a characterization of the biased random walker which will be the subject of a forthcoming paper [16].

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