In an Ising model with spin–exchange dynamics damage always spreads

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Abstract. We investigate the spreading of damage in Ising models with Kawasaki spin–exchange dynamics which conserves the magnetization. We first modify a recent master equation approach to account for dynamic rules involving more than a single site. We then derive an effective-field theory for damage spreading in Ising models with Kawasaki spin–exchange dynamics and solve it for a two-dimensional model on a honeycomb lattice. In contrast to the cases of Glauber or heat-bath dynamics, we find that the damage always spreads and never heals. In the long-time limit the average Hamming distance approaches that of two uncorrelated systems. These results are verified by Monte Carlo simulations.

1. Introduction

Damage spreading (DS) investigates how a small perturbation in a cooperative system changes during the time evolution [1–4] (for a short review see, e.g. [5]). In order to study DS two replicas of the system are considered which evolve stochastically under the same noise realization (i.e. the same random numbers are used in a MC procedure). The difference in the microscopic configurations of the two replicas constitutes the 'damage'. Depending on the Hamiltonian, the dynamic rules, and the external parameters the damage will either spread or heal with time (or remain in a finite spatial region). This behaviour distinguishes chaotic or regular phases.

Kinetic Ising models are among those systems for which DS has been studied most intensively. The majority of the work has been devoted to single-spin–flip dynamic rules such as Glauber, Metropolis or heat-bath dynamics [3–11] but also the Swendson–Wang cluster algorithm has been investigated [12]. It has been found that the properties of DS (e.g. the question whether the damage spreads or heals for a particular model) depend sensitively on the dynamic rule chosen, i.e. DS is uniquely defined only if one specifies the Hamiltonian and the dynamics. (Note that by considering all possible dynamic rules which are consistent with physics of a single replica an unambiguous definition of DS for a particular model can be obtained [13].)

The Glauber, Metropolis or heat-bath algorithms (as well as all other single-spin–flip algorithms) are examples for a dynamics with non-conserved order parameter. There are, however, many physical systems that can be described by kinetic Ising models with order parameter conservation. A prominent example are, e.g. localized electrons where the Ising variables describe the electronic occupation numbers, and the dynamics consists of thermally assisted hops of an electron from one site to another. The simplest order parameter conserving dynamics in an Ising model is the spin–exchange dynamics of Kawasaki [14]. In

this paper we want to investigate DS for this dynamics. To this end we first generalize the master equation approach [10, 11] to dynamic rules involving more than one site. We then derive an effective-field theory for DS in an Ising model with spin–exchange dynamics and solve it for a two-dimensional model on a honeycomb lattice. We find that in this model the damage always spreads. The stationary value of the damage is given by $D^* = (1 - m^2)/2$ (*m* is the magnetization) which corresponds to completely uncorrelated configurations. The results of the effective-field theory are confirmed by Monte Carlo (MC) simulations.

2. Master equation approach

We consider two identical Ising models with N sites described by the Hamiltonians $H^{(1)}$ and $H^{(2)}$ given by

$$H^{(n)} = -\tfrac{1}{2} \sum_{ij} J_{ij} S_i^{(n)} S_j^{(n)} \tag{1}$$

where $S_i^{(n)}$ is an Ising variable with the values ± 1, and $n = 1, 2$ distinguishes the two replicas. J_{ij} is the exchange interaction between the spins which we take to be J for nearest neighbour sites and zero otherwise. The dynamics (also called the Kawasaki dynamics [14]) consists of exchanging spins on nearest-neighbour sites if the probability

$$P = v(\Delta E/2) = \frac{e^{-\Delta E/2T}}{e^{\Delta E/2T} + e^{-\Delta E/2T}} \tag{2}$$

is larger than a random number $\xi \in [0, 1)$. Here ΔE is the energy change due to the exchange of the spins and T denotes the temperature. With this dynamics the total magnetization does not change with time, i.e. it is a conserved quantity.

   Within the master equation approach [10, 11] the simultaneous time evolution of the two replicas is described by the probability distribution

$$P(v_1, \ldots, v_N, t) = \left\langle \sum_{v_i(t)} \prod_i \delta_{v_i, v_i(t)} \right\rangle \tag{3}$$

where $\langle \cdot \rangle$ denotes the average over the noise realizations. The variable v_i with the values $++$, $+-$, $-+$, or $--$ describes the states of the spin pair $(S_i^{(1)}, S_i^{(2)})$. In the case of a spin–exchange dynamics the distribution P fulfils the master equation

$$\frac{\mathrm{d}}{\mathrm{d}t} P(v_1, \ldots, v_N, t) = - \sum_{\langle ij \rangle} \sum_{\mu_i, \mu_j} P(v_1, \ldots, v_i, \ldots, v_j, \ldots, v_N, t) w(v_i, v_j \to \mu_i, \mu_j)$$
$$+ \sum_{\langle ij \rangle} \sum_{\mu_i, \mu_j} P(v_1, \ldots, \mu_i, \ldots, \mu_j, \ldots, v_N, t) w(\mu_i, \mu_j \to v_i, v_j) \tag{4}$$

where $\langle ij \rangle$ denotes all pairs of nearest neighbours and $w(v_i, v_j \to \mu_i, \mu_j)$ is the probability for a transition of the states of the sites i and j from v_i, v_j to μ_i, μ_j. These transition probabilities can be obtained from (2). In table 1 we list all processes $(v_i, v_j \to \mu_i, \mu_j)$ which lead to creation or destruction of damage, the probabilities for these processes will show up in the damage equation of motion later on. An important observation is that damaged sites can be created and destroyed only in pairs. All damage creating processes in table 1 can be transformed into each other by exchanging systems 1 and 2 and sites i and j. Their transition probabilities are therefore also related by symmetry. The same is true for all damage destroying processes. Thus, it is sufficient to calculate only two independent

Table 1. Damage creating and destructing processes for spin–exchange dynamics, all other processes do not change the damage.

Two damaged sites created	$++, --$	$\rightarrow$	$+-, -+$
	$++, --$	$\rightarrow$	$-+, +-$
	$--, ++$	$\rightarrow$	$+-, -+$
	$--, ++$	$\rightarrow$	$-+, +-$
Two damaged sites destroyed	$+-, -+$	$\rightarrow$	$++, --$
	$+-, -+$	$\rightarrow$	$--, ++$
	$-+, +-$	$\rightarrow$	$++, --$
	$-+, +-$	$\rightarrow$	$--, ++$

of the probabilities $w(\nu_i, \nu_j \rightarrow \mu_i, \mu_j)$, e.g.

$$w(++, -- \rightarrow +-, -+) = [v(h_i^{(2)} - h_j^{(2)} + 2J) - v(h_i^{(1)} - h_j^{(1)} + 2J)]$$
$$\times \Theta(h_i^{(1)} - h_j^{(1)} - h_i^{(2)} + h_j^{(2)}) \tag{5a}$$

$$w(+-, -+ \rightarrow ++, --) = [v(h_j^{(2)} - h_i^{(2)} + 2J) - v(h_i^{(1)} - h_j^{(1)} + 2J)]$$
$$\times \Theta(h_i^{(1)} - h_j^{(1)} - h_j^{(2)} + h_i^{(2)}) \tag{5b}$$

where $h_i = \sum_j J_{ij} S_j$ is the local magnetic field of site i.

As in the case of Glauber or heat-bath dynamics we derive an effective-field theory by assuming that fluctuations at different sites are statistically independent which amounts to approximating the distribution $P(\nu_1, \ldots, \nu_N, t)$ by a product of single-site distributions $P_{\nu_i}(t)$. Order parameter conservation in the two systems imposes two conditions: $P_{++}(t) + P_{+-}(t) = $ constant and $P_{++}(t) + P_{-+}(t) = $ constant. Inserting the decomposition

$$P(\nu_1, \ldots, \nu_N, t) = \prod_{i=1}^{N} P_{\nu_i}(t) \tag{6}$$

into the master equation (4) gives a system of coupled equations of motion for the single-site distributions

$$\frac{\mathrm{d}}{\mathrm{d}t} P_{\nu_i} = \sum_{\nu_j, \mu_i, \mu_j} [-P_{\nu_i} P_{\nu_j} W(\nu_i, \nu_j \rightarrow \mu_i, \mu_j) + P_{\mu_i} P_{\mu_j} W(\mu_i, \mu_j \rightarrow \nu_i, \nu_j)] \tag{7}$$

where $W(\nu_i, \nu_j \rightarrow \mu_i, \mu_j)$ is the transition probability w averaged over the states ν of all sites except for i and j. The total damage (Hamming distance) D can be expressed in terms of the single-site distribution P_ν:

$$D = \left\langle \frac{1}{2N} \sum_{i=1}^{N} |S_i^{(1)} - S_i^{(2)}| \right\rangle = P_{+-} + P_{-+}. \tag{8}$$

We note, that in contrast to Ising models with a non-conserved order parameter, the effective-field theory (7) is not very useful in describing a *single* system since the only remaining dynamic variable for a single system, namely m, does not change during the time evolution. The damage is, however, not conserved and (7) constitutes a useful mean-field theory for its time evolution.

From the single-site master equation (7) and table 1 we derive an equation of motion of the damage. Using some symmetry relations [15] between the transition probabilities W, it

reads

$$\frac{d}{dt}D = -2D^2 W(+-, -+ \to ++, --) + 2[(1-D)^2 - m^2]W(++, -- \to +-, -+).$$

(9)

So far the considerations have been valid for all dimensions and lattice types. To proceed we now study a particular system, namely a two-dimensional Ising model on a honeycomb lattice. The same model was studied in [10, 11] for single-spin–flip dynamic rules. The calculation of the average transition probabilities W can be carried out analogously to the case of single-spin–flip dynamics. It is straightforward but tedious, the details will be published elsewhere [15]. Here we only give the results:

$$W(++, -- \to +-, -+) = \left(-\frac{D^4}{2} + D^3 - \frac{3D^2}{4} + \frac{D}{2} - \frac{D^2 m^2}{4} + \frac{Dm^2}{2}\right) t_2$$
$$+ \left(-\frac{D^4}{16} + \frac{D^3}{4} - \frac{3D^2}{8} + \frac{D}{4} + \frac{D^2 m^2}{8} - \frac{Dm^2}{4}\right) t_4$$

(10a)

$$W(+-, -+ \to ++, --) = \left(-\frac{D^4}{2} + D^3 - \frac{3D^2}{4} + \frac{1}{4} - \frac{D^2 m^2}{4} - \frac{m^2}{4}\right) t_2 +$$
$$\left(-\frac{D^4}{16} + \frac{1}{16} - \frac{m^2}{8} + \frac{m^4}{16}\right) t_4.$$

(10b)

Here $t_n = \tanh(nJ/T)$. If we insert (10b) into the damage equation of motion (9) we observe that the death term (first line of equation (9)) is of order D^2 for small D. This is a major difference to the case of Glauber and heat-bath dynamics [10, 11] (where the death term is of order D) and reflects the fact that for spin–exchange dynamics the damage can only be destroyed pairwise. In contrast, the birth term is of order D (as it is for Glauber order heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough D the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is introduced. Thus, m can be taken to be the equilibrium value of the magnetization which is zero for $T > T_c \approx 2.11J$ and

$$m^2 = \frac{\frac{3}{4}(\tanh 3J/T + \tanh J/T) - 1}{\frac{3}{4}\tanh J/T - \frac{1}{4}\tanh 3J/T}$$

(11)

for $T < T_c$ in our effective-field theory [10]. Obviously, $D = D_1^* = 0$ is always a fixed point (FP) of (9). To investigate its stability we expand (9) to linear order in D. The resulting linearized equation of motion is given by $dD/dt = \lambda_1 D$ with

$$\lambda_1 = (1-m^4)\tanh\frac{2J}{T} + \frac{1}{2}(1-m^2)^2 \tanh\frac{4J}{T}.$$

(12)

The Lyapunov exponent λ_1 is always positive, thus the FP D_1^* is always unstable. In figure 1 we show the temperature dependence of λ_1. Since the Hamiltonian and the dynamic rule are invariant under a global flip of all spins, the existence of the FP $D_1^* = 0$ implies the existence of the FP $D_2^* = 1$ with the same stability properties.

In the paramagnetic phase the only other stationary solution of (9) in the physical interval $0 \leqslant D \leqslant 1$ is $D_3^* = \frac{1}{2}$. By expanding (9) around $D = \frac{1}{2}$ we obtain the corresponding Lyapunov exponent,

$$\lambda_3 = -\frac{3}{8}\tanh\frac{2J}{T} - \frac{13}{64}\tanh\frac{4J}{T}.$$

(13)

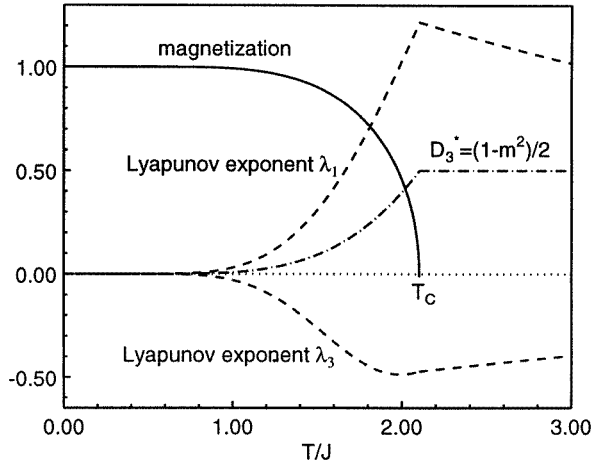**Figure 1.** Results of the effective-field theory for damage spreading in the kinetic Ising model with spin–exchange dynamics.

Since λ_3 is always negative the FP $D_3^* = \frac{1}{2}$ is stable in the entire paramagnetic phase. The temperature dependence of λ_3 is also shown in figure 1.

In the ferromagnetic phase there are two more stationary solutions of (9) in addition to $D_1^* = 0$ and $D_2^* = 1$. If the two systems have the same value of the magnetization, $m^{(1)} = m^{(2)} = m$ we obtain the FP $D_3^* = (1 - m^2)/2$. If the two systems have opposite magnetization $m^{(1)} = -m^{(2)} = m$ we obtain the FP $D_4^* = (1 + m^2)/2$. Since D_3^* and D_4^* are related by a global flip of all spins in one of the systems, they have the same stability properties. The corresponding Lyapunov exponents are given by

$$\lambda_3 = \lambda_4 = \left(-\frac{3}{8} - \frac{m^2}{2} + \frac{m^4}{4} + \frac{m^6}{2} + \frac{m^8}{8} \right) \tanh \frac{2J}{T}$$
$$+ \left(-\frac{13}{64} + \frac{5m^2}{16} + \frac{m^4}{32} - \frac{3m^6}{16} + \frac{3m^8}{64} \right) \tanh \frac{4J}{T}. \tag{14}$$

They are always smaller than zero, thus D_3^* and D_4^* are stable in the entire ferromagnetic phase. The temperature dependence of D_3^* and λ_3 is shown in figure 1.

We now show that at the stable FPs the configurations of the two systems are completely uncorrelated. From the definition (8) of the damage we obtain

$$D = \frac{1}{2N} \sum_{i=1}^{N} \langle |S_i^{(1)} - S_i^{(2)}| \rangle = \frac{1}{2N} \sum_{i=1}^{N} (1 - \langle S_i^{(1)} S_i^{(2)} \rangle). \tag{15}$$

For uncorrelated configurations of $S_i^{(1)}$ and $S_i^{(2)}$ we have $\langle S_i^{(1)} S_i^{(2)} \rangle = \langle S_i^{(1)} \rangle \langle S_i^{(2)} \rangle = \pm m^2$ if the two systems have equal or opposite magnetization, respectively. Thus, for uncorrelated configurations we obtain $D = (1 \mp m^2)/2$. These are exactly the values of D_3^* and D_4^*.

3. MC simulations

We have verified the main predictions of the mean-field theory by MC simulations of a three-dimensional Ising model with Kawasaki spin–exchange dynamics according to (2). The simulations are carried out on cubic lattices with up to $N = 101^3$ sites with periodic
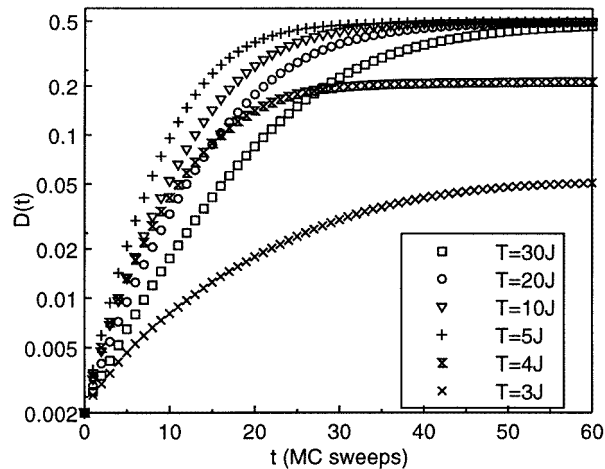
Figure 2. Time evolution of the damage in an Ising model with spin–exchange dynamics. The data points represent averages over 100 runs of a system of 27^3 sites.

boundary conditions. By comparing different system sizes we verify that any finite-size corrections to the results are smaller than the statistical error of the simulation. This is easily possible since we are away from a spreading transition and thus the damage correlation length is finite.

In this study we are not interested in phase separation processes. We thus prepare the system with the correct equilibrium magnetization value for each temperature simulated. 2000 MC sweeps are carried out to equilibrate the system. Then the initial damage D_0 is created by exchanging randomly chosen pairs of nearest-neighbour spins in one of the systems. We use values of D_0 between 5×10^{-4} and 5×10^{-2}. After that both systems evolve in parallel using the same random numbers. Examples of the time evolution of the damage are shown in figure 2. Within the first 5 to 10 MC sweeps the damage increases approximately exponentially with time. A fit of the data to an exponential law gives an estimate for the Lyapunov exponent λ_1. We note that the damage time evolution shows a systematic deviation from an exponential law which manifests in a slight downward curvature in figure 2. This deviation stems from the fact that we are simulating a lattice system. Since with Kawasaki dynamics the damage can spread at most two lattice constants per time step the increase of the damage with time is bounded by a power law, $D(t) \leqslant D_{max} \sim (2t)^3 D_0$. Therefore, a pure exponential spreading can only be observed as long as the probability for any site (or pair of sites) to become damaged during a particular time step is small compared to one. (In this case the above bound set by the lattice does not play a role.) For our system this condition is, however, only fulfilled for small temperatures.

In order to determine the long-time limit of the average damage we average its values over 5000 MC sweeps after a plateau has been reached. The results of our simulations are summarized in figure 3. We indeed find that the FP D_1^* is unstable, and that the damage always spreads. The Lyapunov exponent λ_1 of the FP D_1^* is positive for all temperatures investigated. The asymptotic average damage takes exactly the value of two uncorrelated configurations, namely $D_3^* = (1 - m^2)/2$. (We did not observe the other stable FP $D_4^* = (1 + m^2)/2$ since we always started with the two systems having the same magnetization.)
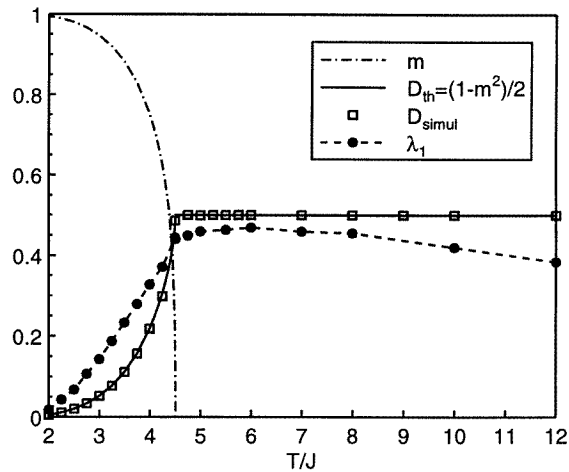
Figure 3. Asymptotic average damage D_3^* and Lyapunov exponent λ_1 for the kinetic Ising model with spin–exchange dynamics. The Lyapunov exponents have been obtained from 100 runs of a 27^3 system. The FP values D_3^* has been calculated from 10 runs of a 101^3 system. Their statistical errors are smaller than the symbol size.

4. Conclusions

To summarize, we have used an effective-field theory and MC simulations to show that the time evolution of a kinetic Ising model with Kawasaki spin–exchange dynamics is chaotic for all temperatures in the sense that the FP $D_1^* = 0$ is unstable. Moreover, we have shown that two systems whose initial configurations differ only at a few sites become completely uncorrelated in the long-time limit. This corresponds to an asymptotic average damage of $D = (1 - m^2)/2$.

In this last part of this paper we wish to discuss how general these results are. Since the properties of DS are known to depend on how the random numbers are used in the update process [13] for single-spin–flip dynamics, an analogous comparison for spin–exchange dynamics is desirable. However, the main properties of our solution will be robust against such changes in the update rules. In particular, the fact that the damage death rate (see equation (9)) is of order D^2 is a result of the spin–exchange mechanism alone. It is therefore independent of how the random numbers are used in the update rule. This suggests that the main finding of this paper, namely that the spin–exchange dynamics is chaotic for all temperatures is valid not only for the Kawasaki update rule (2) but in general. As a first step of a future systematic investigation of different update rules we have studied a modified version of the Kawasaki dynamics. The modification consists of using the random number ξ if the configuration of the spin pair selected for the exchange is $(+-)$ but using $1 - \xi$ instead if the configuration is $(-+)$. This modified update rule can be seen as the spin–exchange analogue of the heat-bath dynamics (in the same sense as the Kawasaki dynamics can be seen as the analogue of the Glauber dynamics). In figure 4 we compare the asymptotic average damage of the Kawasaki and the modified spin–exchange dynamics. The modified dynamics gives lower damage values than the Kawasaki dynamics for all temperatures. Nonetheless, the fixed point $D_1^* = 0$ is unstable for all finite temperatures, and the asymptotic damage is finite. This is in agreement with the above suggestion that a spin–exchange dynamics is always chaotic irrespective of the particular update rule.
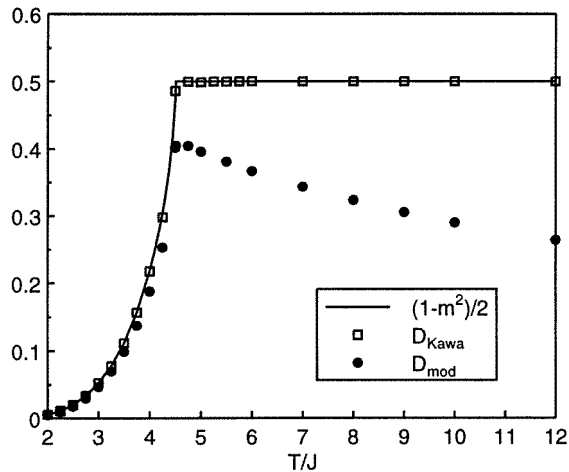
Figure 4. Comparison of the asymptotic average damage D_3^* for the kinetic Ising model with Kawasaki and modified spin–exchange dynamics.

Let us finally discuss the relation of the DS process discussed here with other non-equilibrium processes. As already mentioned, a key feature of DS with spin–exchange dynamics is that damaged sites can heal only in pairs while they can diffuse alone and also create further damage. This is different from the contact process and other processes in the directed percolation universality class where a single active site can die locally with finite probability. There is, however, a simple reaction-diffusion process which should show qualitatively the same behaviour as DS with spin–exchange dynamics. Since for small damage D the birth rate is proportional to D (and since damage is created in pairs) while the death rate is proportional to D^2 (see equations (9), (10)), such a reaction–diffusion process could be defined by the reactions

$$A \xrightarrow{p_1} 3A$$
$$2A \xrightarrow{p_2} 0 \tag{16}$$
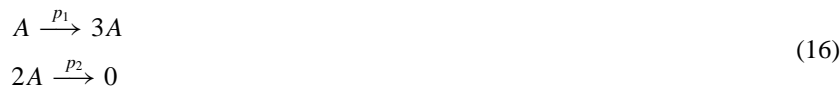
and additional diffusion of the substance A. For small concentrations of A it should have the same qualitative behaviour as DS with spin–exchange dynamics for small damage.

Acknowledgments

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