Damage spreading in the q-state Potts model

Marta F. de A. Bibiano
Departamento de Física, Universidade Federal de Pernambuco, 50670-901 Recife, Pernambuco, Brazil and Departamento de Física, Universidade Federal da Paraíba, 58109-000 Campina Grande, Paraíba, Brazil

F. G. Brady Moreira
Departamento de Física, Universidade Federal de Pernambuco, 50670-901 Recife, Pernambuco, Brazil

A. M. Mariz
Departamento de Física Teórica e Experimental, Universidade Federal do Rio Grande do Norte, 59072-970 Natal, Rio Grande do Norte, Brazil

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Dynamical evolution, in the phase space, of the ferromagnetic q-state Potts model on a square lattice is used in order to study the spread of damage. Our results obtained by numerical Monte Carlo simulation, updating the system by a Glauber dynamics, show that this approach is appropriate to calculate the critical temperature T_c (the same as T_d where the damage spreads), as well as to indicate the order of the phase transition (second-order for $q \leqslant q_c$ and first-order for $q > q_c$). The present simulation on finite systems yields $q_c = 7$, to be compared with the exact value of $q_c = 4$ in the thermodynamical limit. [S1063-651X(97)10402-0]

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Among several models of statistical mechanics employed to study cooperative systems (many degrees of freedom mutually interacting), one of the most useful is the Potts model, developed as a generalization of the Ising model and appropriate to describe many real systems. In this model, the sites of a lattice are occupied by identical variables σ_i, each one having q possible states. The Hamiltonian for the q-state Potts model is given by [1,2]

$$H = -\sum_{\langle i,j \rangle} J_{ij} \delta(\sigma_i, \sigma_j), \tag{1}$$

where $\langle i,j \rangle$ denotes the sum over all pairs of nearest-neighbor sites of the lattice, J_{ij} is the coupling constant, $\delta(\sigma_i, \sigma_j)$ is the Kronecker function, and $\sigma_i = 0,1,2,\ldots,(q-1)$.

On the square lattice, the uniform ferromagnetic model ($J_{ij} = J > 0$) presents a phase transition at the critical temperature $k_B T_c(q)/J = 1/\ln(1+\sqrt{q})$ [3], where k_B is the Boltzmann constant. Most interesting, the order of the phase transition changes from second order for $q \leqslant 4$ to first order for $q \geqslant 5$ [4]; the same phenomenon occurs in the three-dimensional case at the neighborhood of $q \simeq 3$.

As few exact results are known, in one and two dimensions, several methods have been applied in the study of this model as, for example, the renormalization group, series expansion, and numerical simulation [2]. In the latter approach [5,6], time evolution of some configurations of the model, in phase space, is monitored and both equilibrium and nonequilibrium physical quantities can be calculated.

In the last years, a method of numerical simulation that has been proved useful is the so-called damage spreading approach. It consists of following the simultaneous time evolution of two microscopic configurations of the model and of measuring the total damage between them.

The spread of the damage technique has attracted great attention, mainly in the case of models defined in terms of Boolean variables; e.g., the Ising model [7–14] and cellular automata [15]. Some interesting results were noted: (i) there is a dynamical critical phenomenon at the frontier between the (chaotic) region, where the damage spreads, and the (frozen) region, where the damage heals; (ii) surprisingly, this phenomenon is also very sensitive to aspects such as the initial damage, and the dynamical rule used for the system to evolve; (iii) in the case of thermal models there is, in general, good agreement between the critical temperature for damage spreading, T_d, and the Curie critical temperature, T_C.

For the q-state Potts model considered here, we monitor the time evolution of two configurations $A = \{\sigma_i^A(t)\}$ and $B = \{\sigma_i^B(t)\}$, on a square lattice with N sites, and the total average damage at time t is calculated as the fraction of corresponding sites that are in different states, that is,

$$D(t) = \frac{1}{N} \sum_{i=1}^{N} [1 - \delta(\sigma_i^A(t), \sigma_i^B(t))]. \tag{2}$$

Starting with configuration A thermalized at a given temperature T, configuration B is created with a certain fraction $D(0) = M/N$ of damaged sites, as compared with those corresponding sites of A. For each temperature T and initial damage $D(0)$, we then let both configurations evolve in time according to the same dynamics, i.e., the same rule and the same random number sequence in the Monte Carlo procedure. After a relaxation time needed for the damaged copy to also be thermalized, we monitor the damage for a long time in order to calculate its time average value given by the Hamming distance (2). This procedure is repeated for many different samples (initial configurations A and B).

At a given time, the variable $\sigma_i(t) = s$ at site i, is updated according to the following rule: First, the new state

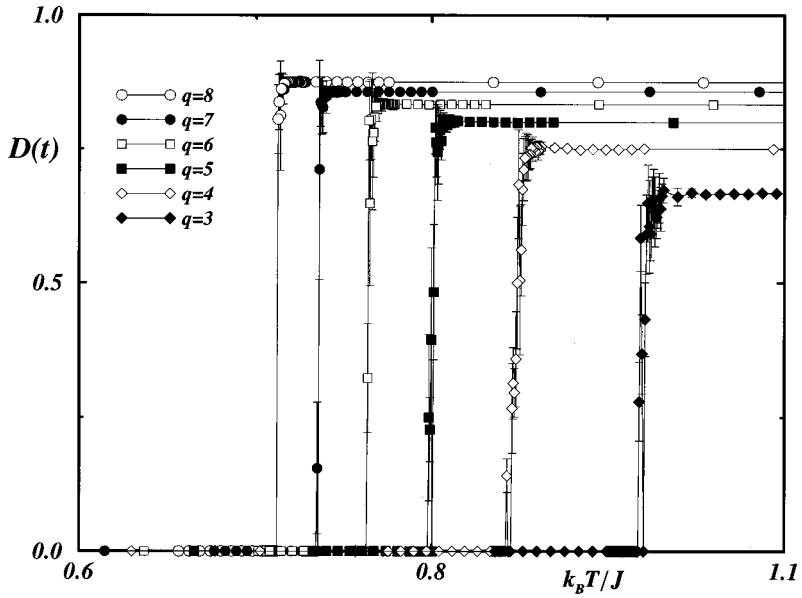

FIG. 1. Average damage $D(t)$ as function of the temperature T for $D(0)=1/N$ and 50×50 lattices, obtained from simulations on the q-state Potts model employing a Glauber dynamics (see text). The damage equals $(q-1)/q$ in the chaotic region.

$\sigma_i(t+1)=s'$, with $(s'\neq s)$, is chosen with equal probability. This is performed on the computer by dividing the interval $[0,1]$ into $(q-1)$ equal pieces, and calling a random number $x_i(t)$ uniformly distributed between 0 and 1. In the present implementation the new state is set equal to s' if $x_i(t)$ falls in the interval

$$\frac{r-1}{q-1}\leqslant x_i(t)<\frac{r}{q-1}, \tag{3}$$

where $r=1,2,\ldots,(q-1)$ and $s'=(s+r)\mathrm{mod}q$.

Second, the state s' is then accepted with probability

$$p_i(t)=\frac{1}{1+\exp(\beta\Delta H)}, \tag{4}$$

where $\beta=1/k_BT$ and ΔH is the change in energy associated with such a move. On the computer, this is implemented by calling a second random number $y_i(t)$ uniformly distributed in the interval $[0,1]$, and setting

$$\sigma_i(t+1)=\begin{cases} s' & \text{if } y_i(t)\leqslant p_i(t) \\ s & \text{otherwise.} \end{cases} \tag{5}$$

The same pair of random numbers $x_i(t)$ and $y_i(t)$ is used for updating $\sigma_i^A(t)$ and $\sigma_i^B(t)$ at site i in both configurations. In the high-temperature limit, where the probabilities given in Eq. (4) go to 0.5 independent of the neighbor configurations, the application of the above dynamical rule to damage spreading simulations yields a vanishing Hamming distance: This corresponds to a generalization of the Glauber dynamics high-temperature result [9] for an Ising $(q=2)$ ferromagnet. It is also important to note that, once the configurations A and B become identical they will always stay identical.

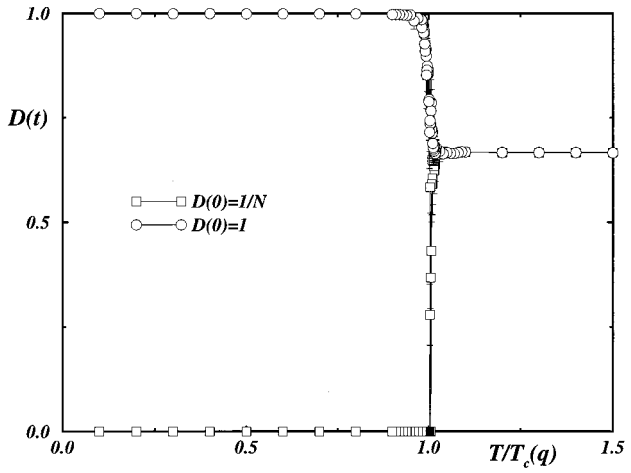

FIG. 2. Average damage $D(t)$ vs the reduced temperature $T/T_c(q)$ for $q=3$ and for initial damages $D(0)=1/N$ and $D(0)=1$. We have observed the same behavior for all values of $q\geqslant 3$; while for $q=2$ an initial symmetric damage is preserved.

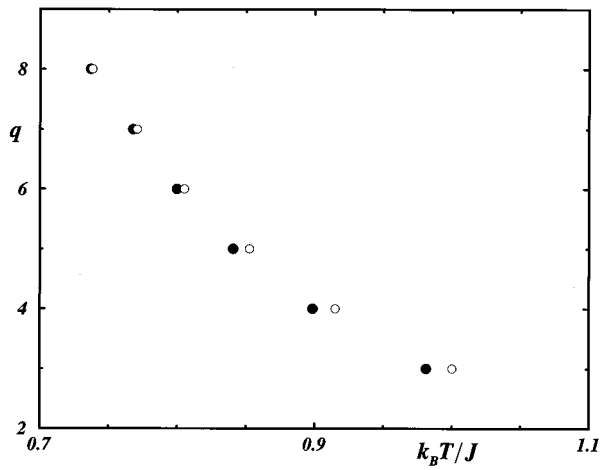

FIG. 3. The q dependence of the temperature T^* (open circles) above which the damage becomes independent of the inital condition, and the dynamic transition temperature T_d (closed circles).

Figure 1 shows the temperature dependence of the long-time damage, obtained from simulations on square lattices of size 50×50 with periodic boundary conditions, and for initial damage $D(0)=1/N$. The damage was allowed to relax over a time of 1000 Monte Carlo steps per spin, its spreading was monitored during 2000 time units. For each temperature the averages were performed over 64 samples. For all values of q, the above dynamics yields a frozen phase for $T<T_d$ and a chaotic phase for $T\geqslant T_d$.

The chaotic phase has a damage rapidily increasing to its high-temperature value $D(T\rightarrow\infty)=(q-1)/q$. At this limit, all q^2 configurations of two corresponding sites occur with equal probability, but only $q(q-1)$ corresponds to damaged configurations.

We have noted for all values of q that $T_d(q)\simeq T_c(q)$ (in the limit of precision of our calculations), showing that this approach can be used to obtain the critical temperature $T_c(q)$ in other lattices where the exact value is not available.

In Fig. 2 we show for $q=3$ the behavior of the average damage for both $D(0)=1/N$ and $D(0)=1$, as a function of the reduced temperature $T/T_c(q)$. In the latter case, the frozen region disappears, but for a characteristic temperature $T^*\geqslant T_d$ the damage assumes its high-temperature value $(q-1)/q$, joining with the curve for $D(0)=1/N$. The same behavior is observed for all values of $q\geqslant3$. We recall that for $q=2$, i.e., for the Ising ferromagnet, the Glauber dynamics preserves the initial symmetric damage, $D(0)=1$, for all times and temperatures.

The temperature T^* above which the average damage becomes independent of its initial condition, allows us to define an interval $\Delta T=T^*-T_d$ whose q dependence shows a decreasing behavior with increasing values of q (see Fig. 3). For $q=8$ we obtain $\Delta T=0.001T_c(q)$, which is the limit of precision of our simulation, characterizing a discontinuous behavior of the temperature dependence of the average damage. The value of $q^*=8$ is here identified with q_c+1, where the system undergoes a first-order phase transition. The estimate value of $q_c=7$ that follows from simulations on lattices of size 50×50, compared with the exact result of $q_c=4$, suggests a weak convergence to the thermodynamical limit. Indeeed, the latent heat increases very slowly with q, for $q>4$ [4]. Further work, addressed to a finite-size analysis of the L dependence of ΔT, would be of interest in order to improve the estimation of the critical q value.

To summarize, our damage spread study on the ferromagnetic q-state Potts model on square lattices, showed that it is possible to calculate the critical temperatures of the model as well as to give some indication of the order of the phase transition.

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