Nonexponential relaxation in fully frustrated models

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We study the dynamical properties of the fully frustrated Ising model. Due to the absence of disorder the model, contrary to spin glass, does not exhibit any Griffiths phase, which has been associated to nonexponential relaxation dynamics. Nevertheless, we find numerically that the model exhibits a stretched exponential behavior below a temperature T_p corresponding to the percolation transition of the Kasteleyn-Fortuin clusters. We have also found that the critical behavior of these clusters for a fully frustrated q-state spin model at the percolation threshold is strongly affected by frustration. In fact while in the absence of frustration the $q=1$ limit gives random percolation, in the presence of frustration the critical behavior is in the same universality class of the ferromagnetic $q=1/2$-state Potts model. [S1063-651X(97)02110-7]

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I. INTRODUCTION

Glassy systems at low temperatures undergo a transition characterized by the freezing of structural relaxation, in which the system is trapped in a disordered metastable configuration. Already at temperatures higher than the ideal glass transition temperature T_0, a number of dynamic anomalies are observed. One of these anomalies concerns the relaxation functions of the system, which at high temperatures are characterized by a single exponential. Below some temperature T^* higher than T_0, the long time regime of correlation functions, called α relaxation, is well approximated by a Kohlrausch-Williams-Watts function, also known as ''stretched exponential,''

$$f(t)=f_0\ \exp-(t/\tau)^{\beta}. \tag{1}$$

This behavior has been observed in many real glasses, such as ionic conductors, supercooled liquids, and polymers [1–7].

A similar behavior has been observed in canonical metallic and insulating spin glasses, investigated by neutron and hyperfine techniques [8–13]. These systems can be described by an Ising model, in which ferromagnetic and antiferromagnetic interactions are distributed in a disordered way on the edges of the lattice. The Ising spin glass undergoes a transition at some temperature T_{SG}, called the spin glass transition, analogous to the freezing transition of real glasses. Moreover, as in glass-forming systems, one observes a temperature value $T^*>T_{SG}$ where nonexponential relaxation functions appear. This has been observed for the Ising spin glass in two dimensions (2D) by McMillan [14], and in 3D by Ogielski [15].

Several mechanisms have been proposed to explain the onset of nonexponential relaxation functions like Eq. (1) in spin glasses, when the system approaches the glass transition from above. Randeria *et al.* [16] suggest that the temperature T^* coincides with T_c, the critical temperature of the ferromagnetic model. They base their conjecture on the presence, in the spin glass, of nonfrustrated ferromagnetic-type clusters of interactions, the same that are responsible for the Griffiths singularity [17]. The presence of nonexponential relaxation in this approach is therefore a direct consequence of the quenched disorder.

On the other hand, it has been suggested [18–20] that in the spin glass the onset of stretched exponential relaxation functions may coincide with the percolation temperature T_p of the Kasteleyn-Fortuin and Coniglio-Klein clusters [21,22]. These clusters can be obtained by introducing a bond with probability $p_B=1-e^{-2J/k_BT}$ between nearest-neighbor pairs of spins satisfying the interaction. In the spin glass the percolation threshold of these clusters is higher than T_{SG} [23]. Moreover Stauffer [24] observes nonexponential relaxation in the $d=2$ ferromagnetic Ising model, simulated by conventional spin flip, for temperatures lower than the critical temperature T_c, which coincides with the percolation temperature T_p. In $d=3$ this behavior disappears, and the relaxation is purely exponential for all the temperatures.

To gain more insight into the mechanisms which lead to the appearance of anomalies in the dynamical behavior, in this paper we study the fully frustrated Ising model [25–27] on a bidimensional square lattice, using the conventional spin flip techniques. In this model ferromagnetic and antiferromagnetic interactions are distributed in a regular way on the lattice (see Fig. 1), so that no unfrustrated cluster of interactions exists. Therefore in this model the appearance of a stretched exponential in the relaxation functions cannot be due to the mechanism of Randeria *et al.* We in fact find that the onset of stretched exponentials occurs at the percolation temperature T_p, as we show in Sec. II.

The fully frustrated Ising model can be mapped onto a fully frustrated q-bond percolation by applying the Kasteleyn-Fortuin and Coniglio-Klein cluster formalism, where $q=2$ is the multiplicity of the spins (see Sec. III). This model, which can be generalized to any value of q, is suitable to describe systems with geometrical frustration, and may give insight into the origin of the long relaxation decay in glasses, characterized by stretched exponentials [28]. We study the dynamics of this geometrical model for $q=1$ and $q=2$, using the ''bond flip'' dynamics that will be described in Sec. IV. We find again that the onset of stretched exponentials starts at the percolation transition T_p (Sec. VI).

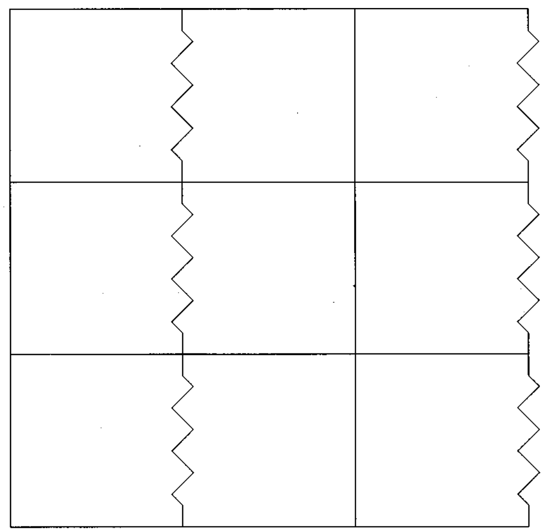

FIG. 1. Distribution of interactions for the fully frustrated model. Straight lines and wavy lines correspond, respectively, to $\epsilon_{ij}=1$ and $\epsilon_{ij}=-1$.

Moreover we also find that the percolation transition is in the same universality class as the $q/2$-state ferromagnetic Potts model, as we show in Sec. V, in agreement with the expectation based on renormalization group [29].

These results thus suggest that the presence of a percolation-type transition may be responsible for the appearance of the ''large scale'' effects of frustration, among which there is the onset of various dynamical anomalies, such as stretched exponential relaxation functions [30,20].

In the frustrated q-bond percolation, the frustration is present at all length scales. To probe the effect of frustration we have modified the model in such a way that only loops of length 4 are considered frustrated (Sec. VII). We find that the model for $q=1$ has the same critical exponents as the ferromagnetic Potts model with spin multiplicity $q=1$ (the random bond percolation model). Namely, this local frustration does not change the critical behavior compared with the unfrustrated model. At the same time, although the dynamics of the model is influenced by the frustration constraint, in the long time regime the relaxation is purely exponential.

II. THE RELAXATION FUNCTIONS OF THE FULLY FRUSTRATED ISING SPIN MODEL

We simulate by conventional spin flip the fully frustrated Ising spin model, defined by the Hamiltonian

$$\mathcal{H}=-J\sum_{\langle ij\rangle}(\epsilon_{ij}S_iS_j-1), \tag{2}$$

where ϵ_{ij} are quenched variables which assume the values ± 1. The ferromagnetic and antiferromagnetic interactions are distributed in a regular way on the lattice (see Fig. 1).

We calculate the relaxation functions of the energy. Averages were made over 32 different random number generator seeds, and between 8×10^5 and 1.8×10^6 steps for acquisition were taken, after 10^4 steps for thermalization, on a system of size $L=64$. Here a unit of time is considered to be one Monte Carlo step, that is, L^2 single spin update trials.

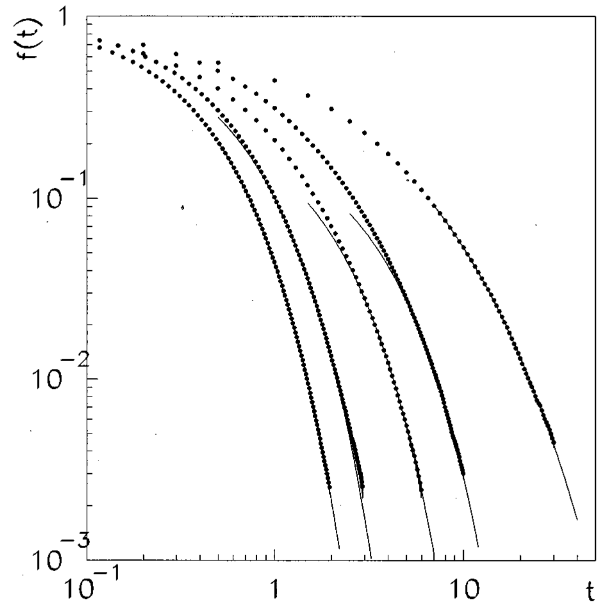

FIG. 2. Relaxation functions $f(t)$ of energy as a function of time t for the fully frustrated Ising model, with spin flip dynamics, lattice size $L=64$, for temperatures (from left to right) $T=11.0,4.5,2.269,1.701,1.110$.

In Fig. 2 we show the results for $T=11.0,4.5,2.269,1.701,1.110$, where temperatures are expressed in units of J/k_B. We observe a two step decay also for very high temperatures. For all the temperatures except $T=11.0$ we fit only the long time tail of the relaxation functions. For temperatures $T>T_p=1.701$ we could fit the long time regime a pure exponential, that is, $\beta=1$ within the errors in Eq. (10). On the other hand, for $T=1.110<T_p$ the long time behavior is not purely exponential, but can be fitted asymptotically with a stretched exponential. In Fig. 3 we show the values of $\beta(T)$ in function of T/T_p.

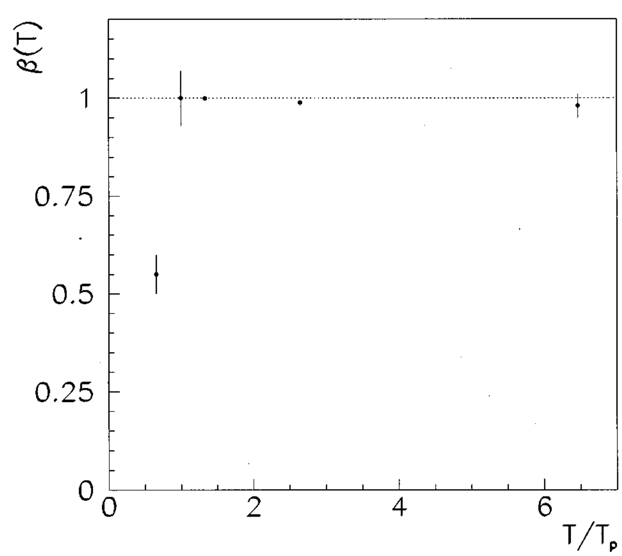

FIG. 3. Stretching exponents $\beta(T)$ as a function of T/T_p, the ratio of temperature over percolation temperature, for the fully frustrated Ising model, with spin flip dynamics, lattice size $L=64$.

III. THE "q-BOND FRUSTRATED PERCOLATION" MODEL

Using the Kasteleyn-Fortuin [21] and Coniglio-Klein [22] cluster formalism for frustrated spin Hamiltonians [23], it is possible to show that the partition function of the model Hamiltonian (2) is given by

$$Z=\sum_{C}{}^{*}e^{\beta\mu n(C)}q^{N(C)}, \tag{3}$$

where $q=2$ is the multiplicity of the spins, $\beta=1/k_BT$, $\mu=k_BT\ \ln(e^{q\beta J}-1)$, and $n(C)$ and $N(C)$ are, respectively, the number of bonds and the number of clusters in the bond configuration C. The summation Σ_C^* extends over all the bond configurations that do not contain a "frustrated loop," that is, a closed path of bonds which contains an odd number of antiferromagnetic interactions. Note that there is only one parameter in the model, namely, the temperature T, ranging from 0 to ∞. The parameter μ, which can assume positive or negative values, plays the role of a chemical potential.

Varying q we obtain an entire class of models differing by the "multiplicity" of the spins, which we call the q-bond fully frustrated percolation model. More precisely, for a general value of q, the model can be obtained from a Hamiltonian [31]

$$\mathcal{H}=-sJ\sum_{\langle ij\rangle}[(\epsilon_{ij}S_iS_j+1)\delta_{\sigma_i\sigma_j}-2], \tag{4}$$

in which every site carries two types of spin, namely, an Ising spin and a Potts spin $\sigma_i=1,\ldots,s$ with $s=q/2$. For $q=1$ the factor $q^{N(C)}$ disappears from Eq. (3), and we obtain a simpler model in which the bonds are randomly distributed under the conditions that the bond configurations do not contain a frustrated loop. For $q\to 0$ we recover the tree percolation, in which all loops are forbidden, be they frustrated or not [32].

When all the interactions are positive (i.e., $\epsilon_{ij}=1$) the sum in Eq. (3) contains all bond configurations without any restriction. In this case the partition function coincides with the partition function of the ferromagnetic q-state Potts model, which in the limit $q=1$ gives the random bond percolation.

From renormalization group and numerical results we expect that the model (3) exhibits two critical points [29,33], the first at a temperature $T_p(q)$, corresponding to the percolation of the bonds on the lattice, in the same universality class of the ferromagnetic $q/2$-state Potts model, and the other at a lower temperature $T_0(q)$, in the same universality class as the fully frustrated Ising model. In the bidimensional case $T_0(q)=0$ [25–27].

IV. MONTE CARLO DYNAMICS

A particular configuration of the model defined by Eq. (3) is determined by the state of each edge between two nearest-neighbor sites, that can be empty or occupied by a bond. The dynamics of the model is carried out in the following way: (i) choose at random a particular edge on the lattice; (ii) calculate the probability P of changing its state, that is, of creating a bond if the edge is empty, and of destroying the bond if the edge is occupied; (iii) change the state of the edge with probability P.

The point (ii) needs the knowledge of a nonlocal property, namely, if a bond placed on the chosen edge closes a loop or not, and if the loop is frustrated or not. This is accomplished in the following way: starting from the two sites at the extremes of the edge, visit the clusters of sites connected to them by a continuous path of bonds; if the clusters collide the bond closes a loop, otherwise it does not. By keeping track of the number of antiferromagnetic bonds traversed visiting the cluster, one can determine also if the loop is frustrated or not.

Note that at high temperatures clusters are small, and are visited in a few iterations, while at low temperatures density of bonds is high, and the clusters collide in a few iterations as well. On the other hand, at the percolation transition clusters are very ramified, and one often must visit a large number of sites before the iteration is over. This makes the algorithm CPU consuming at the percolation transition, and prevents the simulation of very large systems.

From Eq. (3), the statistical weight of a bond configuration C is given by $W(C)=e^{\beta\mu n(C)}q^{N(C)}$ if C does not contain a frustrated loop, and $W(C)=0$ if it does. Thus the transition probabilities for the principle of detailed balance must satisfy

$$P(C\to C')=P(C'\to C)e^{\beta\mu\delta n}q^{\delta N}, \tag{5}$$

where $\delta n=n(C')-n(C)$ and $\delta N=N(C')-N(C)$. Note that from Euler's equation $\delta N=\delta\kappa-\delta n$, where $\delta\kappa=\kappa(C')-\kappa(C)$, and $\kappa(C)$ is the number of loops in configuration C, we can calculate δN knowing δn and $\delta\kappa$. One can easily see that a possible choice for the transition probability $P(C\to C')$ is given by

$$P(C\to C')=\begin{cases}\min(1,e^{\beta\mu\delta n}q^{\delta N}) & \text{if } C' \text{ is not frustrated}\\ 0 & \text{if } C' \text{ is frustrated.}\end{cases} \tag{6}$$

The procedure described above in the points (i)–(iii) is called a "single update trial." A Monte Carlo step consists in $\mathcal{G}$ single update trials, where $\mathcal{G}$ is the total number of edges on the lattice, namely, on the square bidimensional lattice, $\mathcal{G}=2L^2$. In Secs. VI and VII, when we plot relaxation functions of the fully frustrated and locally frustrated bond percolation model, a unity of time is considered to be $\mathcal{G}\langle\rho\rangle^{-1}$ single update trials, or $\langle\rho\rangle^{-1}$ Monte Carlo steps, where $\langle\rho\rangle$ is the average density of bonds, ranging in the interval (0,1).

V. STATIC PROPERTIES

In this section we analyze the percolation properties of the model defined by Eq. (3), for $q=1$ and $q=2$, on a bidimensional square lattice, with fully frustrated interactions. We have used the histogram method for analyzing data [34]. For each value of q, we have simulated the model for lattice sizes $L=32,48,64$. For each size we have considered ten temperatures around the percolation point, taking 10^4 steps for thermalization and between 3×10^5 and 8×10^5 steps for acquisition of histograms. At every step we evaluate the following quantities: density of bonds ρ; existence of a spanning cluster P_∞; mean cluster size χ.

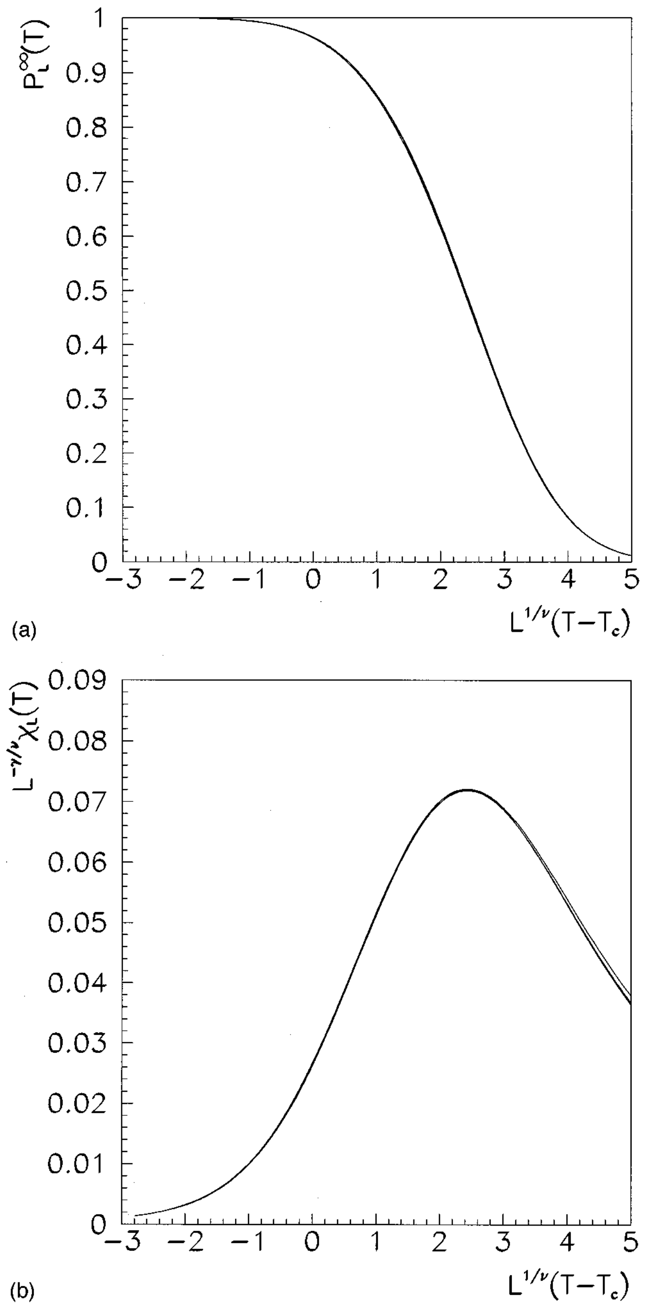

FIG. 4. Finite size scaling of (a) $P_\infty(T)$ and (b) $\chi(T)$, for the $q=1$ model, and for lattice sizes $L=32,48,64$. Curves are indistinguishable in this plot.

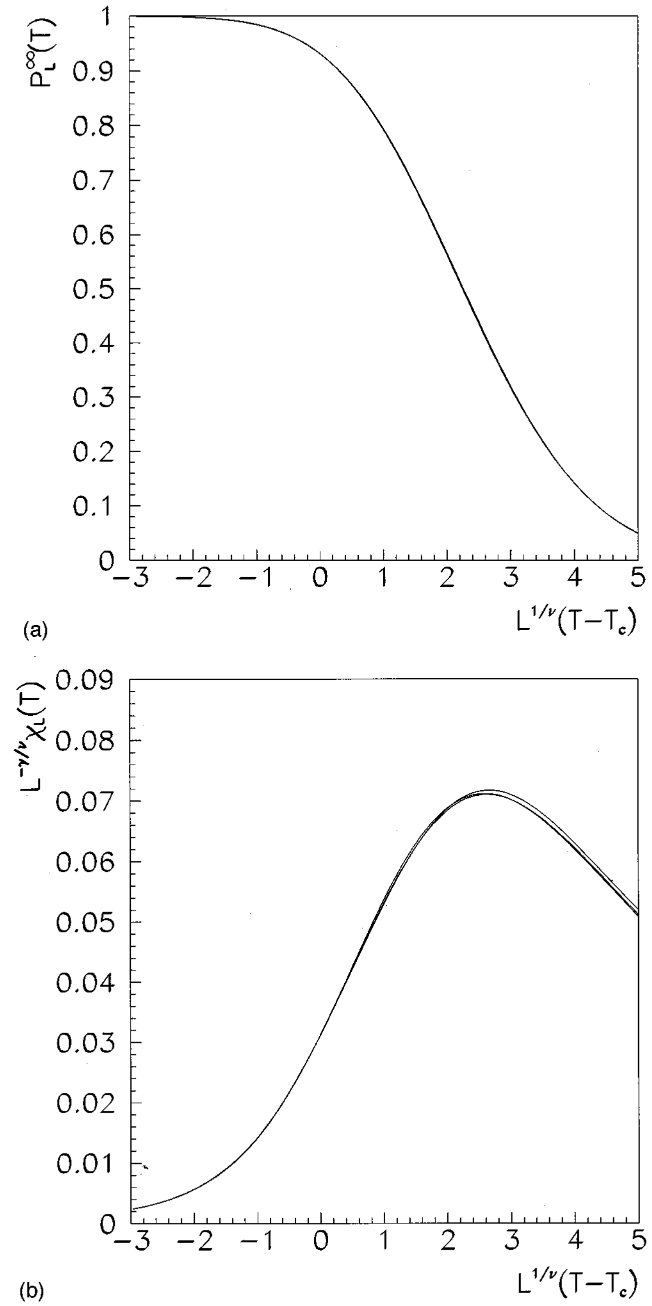

FIG. 5. Finite size scaling of (a) $P_\infty(T)$ and (b) $\chi(T)$, for the $q=2$ model, and for lattice sizes $L=32,48,64$. Curves are indistinguishable in this plot.

The quantity P_∞ assumes the value 1 if the bond configuration percolates, and 0 if it does not. The mean cluster size is defined as [35]

$$\chi=\frac{1}{\mathcal{N}}\sum_s s^2 n_s, \tag{7}$$

where n_s is the number of clusters having size s on the lattice, and $\mathcal{N}=L^2$ is the number of sites. The histogram method allows us to evaluate the thermal averages of these quantities over an entire interval of temperature. The average of the quantity P_∞ is the probability of occurrence of a spanning cluster.

Around the percolation temperature, the averaged quantities $P_\infty(T)$ and $\chi(T)$, for different values of the lattice size L, should obey the finite size scaling [36]

$$P_\infty(T)=F_\infty[L^{1/\nu}(T-T_p)], \tag{8a}$$

$$\chi(T)=L^{\gamma/\nu}F_\chi[L^{1/\nu}(T-T_p)], \tag{8b}$$

where γ and ν are critical exponents of mean cluster size and connectivity length, and F_∞ and F_χ are universal functions. Thus we can fit the values of ν, γ, and T_p so that plotting $P_\infty(T)$ and $L^{-\gamma/\nu}\chi(T)$ as a function of $L^{1/\nu}(T-T_p)$, the functions corresponding to different values of L collapse, respectively, on the universal master curves $y=F_\infty[x]$ and

TABLE I. Critical exponents $1/\nu$ and γ, and percolation transition temperature T_p of the fully frustrated q-bond percolation model with $q=1$, 2, and of the locally frustrated bond percolation model with $\lambda_0=4$.

Model	$1/\nu$	γ	T_p
$q=1$	0.56 ± 0.02	3.22 ± 0.07	1.067 ± 0.001
$q=2$	0.75 ± 0.03	2.34 ± 0.06	1.701 ± 0.001
Local ($\lambda_0=4$)	0.75 ± 0.03	2.33 ± 0.04	1.277 ± 0.001

$y=F_\chi[x]$. Figures 4 and 5 show the data collapse obtained for the $q=1$ and $q=2$ models, for lattice sizes $L=32,48,64$.

The values of the critical exponents extracted from the fit coincide, within the errors, with those of the ferromagnetic Potts model with spin multiplicity $q/2$ [32]. Results are summarized in Table I, while in Table II we report the critical exponents and transition temperature of the ferromagnetic Potts model.

VI. THE RELAXATION FUNCTIONS OF THE "q-BOND FRUSTRATED PERCOLATION" MODEL

In this section we analyze the dynamical behavior of the model defined by Eq. (3), simulated by the algorithm described in Sec. IV. For each temperature T and value of q, 32 different runs were made, varying the random number generator seed, on a system of size $L=64$. We took between 10^3 and 10^4 steps for thermalization, and between 10^5 and 10^6 steps for acquisition, calculating at each step the density of bonds $\rho(t)$. The relaxation function of the density of bonds is defined as

$$f(t)=\frac{\langle\,\delta\rho(t)\,\delta\rho(0)\rangle}{\langle(\delta\rho)^2\rangle}, \tag{9}$$

where $\delta\rho(t)=\rho(t)-\langle\rho\rangle$. For each value of T and q, we averaged the 32 functions calculated, and evaluated the error as a standard deviation of the mean. As we mentioned in Sec. IV, we consider a unit of time to consist of $\mathcal{G}\langle\rho\rangle^{-1}$ single update trials, where $\mathcal{G}=2L^2$ is the number of edges on the lattice.

In Fig. 6 the results for $q=1$, $T=1.440,1.067,0.801,0.625$ are shown. Note that $T_p=1.067$ corresponds to the percolation transition of the model. For $T>T_p$ we fitted the calculated points with the function

$$f(t)=f_0\ \exp[-(t/\tau)^\beta]. \tag{10}$$

The value of β extracted from the fit is equal to one within the error. Thus for $T\geqslant T_p$ the relaxation is purely exponential. For $T<T_p$, we observe a two step decay, and only the long time regime of the relaxation functions could be fitted by Eq. (10). The value of β extracted is less than one, showing that stretched exponential relaxation has appeared for these temperatures. In Fig. 7 the values of $\beta(T)$ as a function of the the ratio T/T_p are shown, with least squares estimation errors.

In Fig. 8 the results for $q=2$, $T=2.269,1.701,1.440,1.110$ are shown. Temperature $T_p=1.701$ corresponds to the percolation transition. The fits were made in the same way described for $q=1$, and the values of $\beta(T)$ extracted are shown in Fig. 9. Also in this case $\beta=1$ within the error for $T\geqslant T_p$, and $\beta<1$ for $T<T_p$. Note that the $q=2$ fully frustrated

TABLE II. Critical exponents $1/\nu$ and γ, and critical temperature T_c of the ferromagnetic Potts model, with multiplicity of spins $q=1/2$, 1, 2.

Model	$1/\nu$	γ	T_c
$q=1/2$	0.56	3.27	1.233
$q=1$	0.75	2.39	1.443
$q=2$	1	1.75	2.269

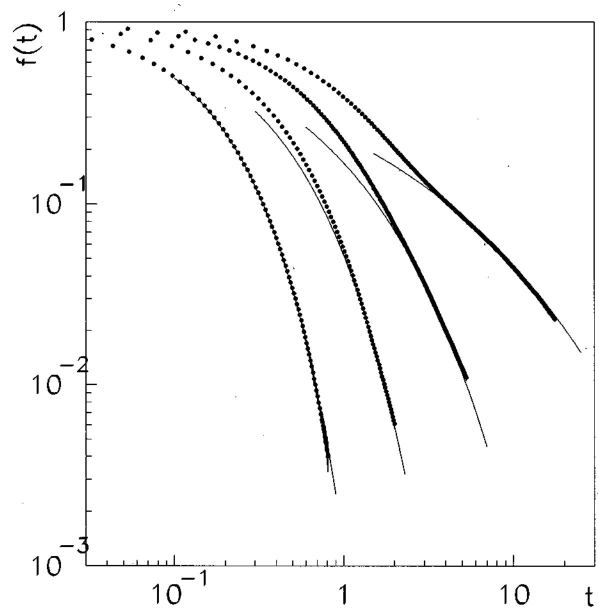

FIG. 6. Relaxation functions $f(t)$ of bond density as a function of time t for $q=1$, lattice size $L=64$, for temperatures (from left to right) $T=1.440,1.067,0.801,0.625$.

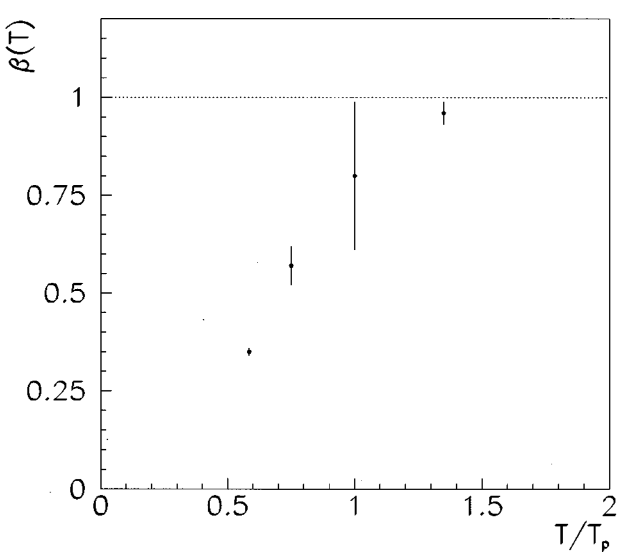

FIG. 7. Stretching exponents $\beta(T)$ as a function of T/T_p, the ratio of temperature over percolation temperature, for the $q=1$ fully frustrated bond percolation model, lattice size $L=64$.

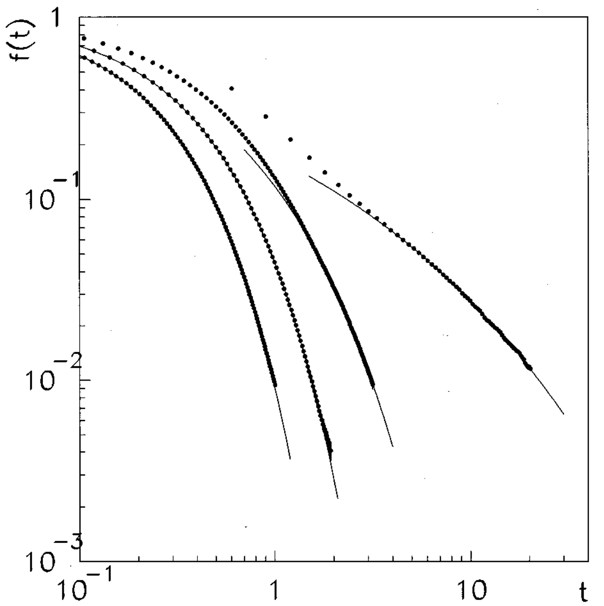

FIG. 8. Relaxation functions $f(t)$ of bond density as a function of time t for $q=2$, lattice size $L=64$, for temperatures (from left to right) $T=2.269, 1.701, 1.440, 1.110$.

bond percolation model can be mapped exactly onto the fully frustrated Ising spin model, as we showed in Sec. III. So it is interesting to compare the relaxation functions of this model to those of the corresponding fully frustrated Ising model, simulated by standard spin flip techniques.

VII. THE LOCALLY FRUSTRATED BOND PERCOLATION

In the fully frustrated q-bond percolation model, the configurations of bonds which contain at least one frustrated loop have zero weight. The size of frustrated loops has no upper limit. To study systematically the effect of frustration, we consider now a modified version of the model, in which

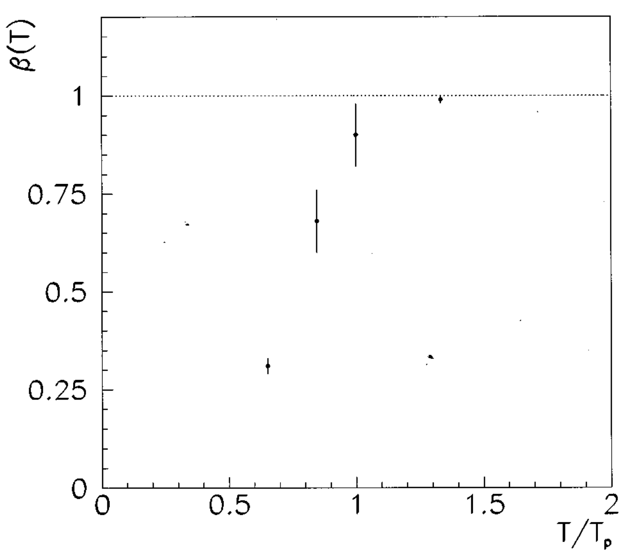

FIG. 9. Stretching exponents $\beta(T)$ as a function of T/T_p, the ratio of temperature over percolation temperature, for the $q=2$ fully frustrated bond percolation model, lattice size $L=64$.

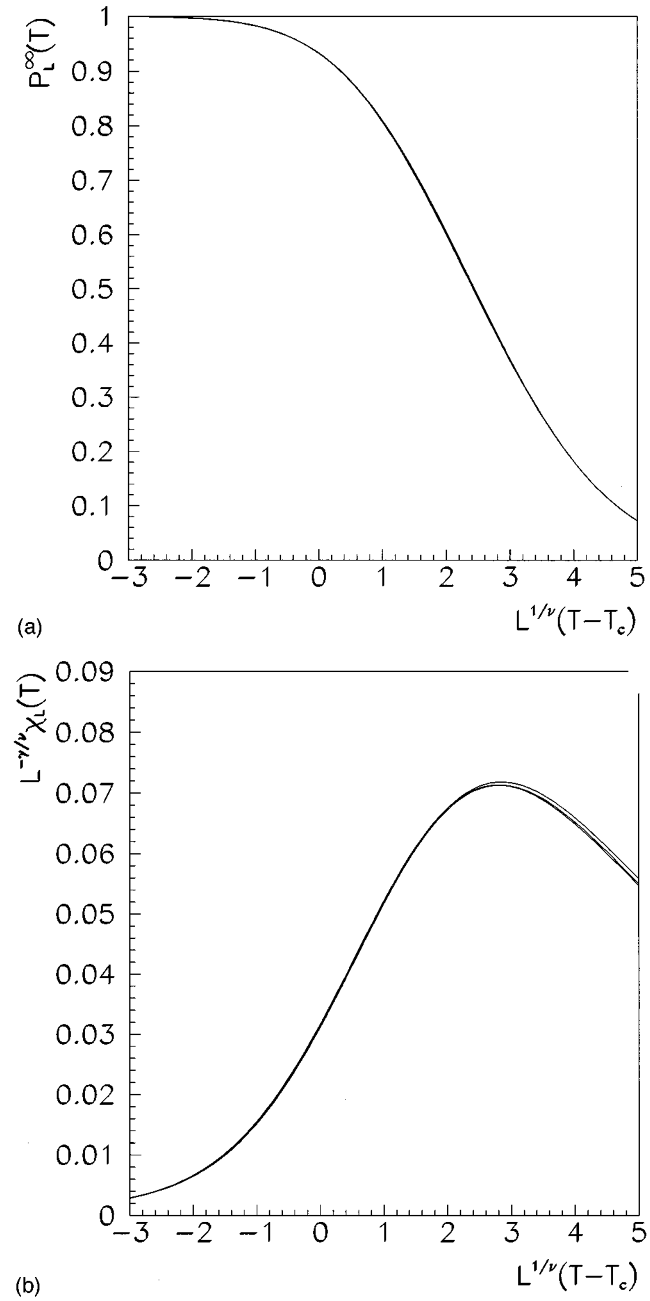

FIG. 10. Finite size scaling of (a) $P_\infty(T)$ and (b) $\chi(T)$, for the local frustrated model, and for lattice sizes $L=32,48,64$. Curves are indistinguishable in this plot.

only loops up to some specified length are considered frustrated, while longer ones are permitted. The partition function of this model is given by

$$Z=\sum_C{}^{(\lambda_0)} e^{\beta\mu n(C)}. \tag{11}$$

Here the parameters β and μ have the same meaning as in Eq. (3), $n(C)$ is the number of bonds in the configuration C, and the sum $\Sigma_C^{(\lambda_0)}$ is extended over the bond configurations that do not contain frustrated loops of length $\lambda \leqslant \lambda_0$. Thus the model switches continuously from the random bond percolation $(\lambda_0=0)$, and the q-bond frustrated percolation with $q=1$ $(\lambda_0=\infty)$.

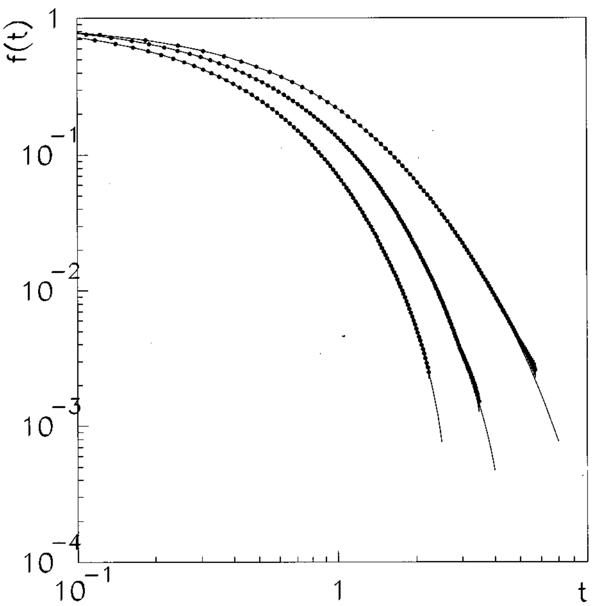

FIG. 11. Relaxation functions $f(t)$ of bond density as a function of time t for the local frustrated model, lattice size $L=64$, for temperatures (from left to right) $T=1.277,0.911,0.625$.

We have studied the critical properties of the model, for $\lambda_0=4$, and its dynamical behavior above and below the percolation transition. The critical exponents extracted from the finite size scaling data collapse (see Fig. 10) coincide within the errors with those of the random bond percolation, as shown in Table I. The percolation temperature is $T_p=1.277$, intermediate between that of the random bond percolation, $T_p=1.443$, and that of the $q=1$-bond frustrated percolation, $T_p=1.067$.

The dynamics, on the other hand, is affected by the local constraint constituted by the frustration, as the autocorrelation functions do not decay as a single exponential when the temperature is lowered below the percolation threshold. However, the long time regime of the relaxation functions could be fitted with an exponential for all the temperatures considered.

In Fig. 11 we show the bond density autocorrelation functions, evaluated on a lattice $L=64$, for temperatures $T=1.277,0.911,0.625$. The function calculated for $T=1.701$ is not shown because it overlaps with the function calculated for $T=1.277$. Solid curves show fits made by a pure exponential. Averages were taken over 32 different runs, each one taking 10^4 steps for thermalization, and between 2×10^5 and 3×10^5 steps for acquisition.

VIII. CONCLUSIONS

We have studied the fully frustrated Ising model and the fully frustrated percolation model. The dynamics of the models was analyzed in detail, in connection with the problem of the onset of stretched exponentials in frustrated systems, like glasses and spin glasses.

Due to absence of disorder in these models, the arguments suggested by Randeria *et al.*, which predict a nonexponential relaxation below the critical temperature T_c of the corresponding ferromagnetic model, do not apply. In fact our results show no sign of complex dynamical behavior at T_c. We find instead an exponential relaxation above the percolation temperature $T\geqslant T_p$, while for $T<T_p$ the long time tail of the relaxation functions can be fitted with a stretched exponential. So we conclude that at least in the models without disorder the appearance of complex dynamics is related to a percolation transition. In systems like spin glasses T_p and T_c are very close, and it is difficult to distinguish numerically where the onset of nonexponential relaxation occurs.

We also find that frustration plays an important role in the critical properties at the percolation threshold T_p. For example, for $q=1$ the critical behavior is in the same universality as the ferromagnetic $q=1/2$-state Potts model, contrary to the unfrustrated case, which corresponds to random bond percolation and is in the same universality class as the $q=1$ ferromagnetic Potts model.

We have also considered a model, the locally frustrated bond percolation, in which only loops up to length 4 are considered frustrated. The model shows the same critical properties as the random bond percolation, showing that the frustration is ''too local'' to change the universality class. Similarly, the relaxation functions in the long time regime can always be fitted with an exponential, showing that the frustration constraint is not enough to give rise to stretched exponential relaxation. More careful study of this model, possibly varying the ''range'' of the frustration between the size of the single *plaquette*, and that of the whole system, may shed more light on the role played by the frustration in the dynamics of complex systems.

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