Potts fully frustrated model: Thermodynamics, percolation, and dynamics in two dimensions

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We consider a Potts model diluted by fully frustrated Ising spins. The model corresponds to a fully frustrated Potts model with variables having an integer absolute value and a sign. This model presents precursor phenomena of a glass transition in the high-temperature region. We show that the onset of these phenomena can be related to a thermodynamic transition. Furthermore, this transition can be mapped onto a percolation transition. We numerically study the phase diagram in two dimensions (2D) for this model with frustration and *without* disorder and we compare it to the phase diagram of (i) the model with frustration *and* disorder and (ii) the ferromagnetic model. Introducing a parameter that connects the three models, we generalize the exact expression of the ferromagnetic Potts transition temperature in 2D to the other cases. Finally, we estimate the dynamic critical exponents related to the Potts order parameter and to the energy.

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I. INTRODUCTION

The glass transition temperature T_g for liquids is defined experimentally as the onset of calorimetric anomalies [1]. It is usually understood that T_g is not related to a thermodynamic transition [2], but to the slowing down of one or more degrees of freedom. This slowing down prevents the system from reaching equilibrium [3,4]. This question is of interest because almost all liquids can form glasses if cooled at a high enough rate. Moreover, many other materials such as, for example, polymers, microemulsions, granular material, vortex glasses, ionic conductors, colloids, plastic glassy crystals, and spin glasses (SGs) [5], show glassy properties.

Even well above T_g, where glassy systems actually can equilibrate, they show experimentally dynamic anomalies as precursor phenomena of the glass transition [3,6–8]. From a theoretical point of view, one of the open questions is if these precursor phenomena are related to the thermodynamics of the system [2,4,9,10], or if they are not, like the glass transition occurring at lower temperature T_g. In particular, for the Ising SG [5] such a relation between precursor phenomena and a thermodynamic free energy *essential* singularity has been shown [9,11,12]. Indeed, in this model there is a dynamic anomaly at a temperature T^*. Above T^* the relaxation processes have an exponential behavior, while below T^* they have a nonexponential behavior. Theoretical and numerical evidence shows that T^* coincides with the Griffiths temperature T_c [11]. This T_c is the transition temperature that the model would have if the frustration due to disorder were removed. A way to remove the frustration is, for example, to substitute every antiferromagnetic interaction with a ferromagnetic interaction. In general, on removing the frustration, the model will have ferromagnetic regions and antiferromagnetic regions and T_c will be the transition temperature of the unfrustrated model. To be more precise, the free energy of the Ising SG in an external field has a singularity which disappears in the limit of zero external field and which occurs at a temperature that goes to T_c in the same limit. This singularity is present only in disordered systems. The relation $T^*=T_c$ has also been shown to be valid numerically in two dimensions (2D) for a model with Potts variables that generalizes the Ising SG [13]. This generalized model will be considered in the following and we will refer to it as the Potts SG.

Until now we talked about glass dynamics in systems with disorder, but numerical simulations show that it is possible to observe glassy behavior with precursor phenomena for spin systems *without* disorder but *with* frustration [14,15]. These systems, due to the lack of disorder, are more suitable for a theoretical approach [16,17]. In particular, one can try to answer the question about the relation between the precursor phenomena and the thermodynamics of the system.

In Ref. [14] a simple case was considered: the fully frustrated (FF) Ising model [19] where ferromagnetic and antiferromagnetic interactions are ordered in such a way that any lattice cell has an odd number of antiferromagnetic interactions (i.e., is frustrated). It is shown (by simulations in 2D and 3D) that the onset T^* of nonexponential relaxation processes is related to a random-bond percolation transition [14]. As for the Ising SG, it is possible to generalize the FF Ising model to a FF model with Potts variables [13]: the Potts FF model that will be described in detail in the following. In Ref. [13] the dynamics of the Potts FF model was compared with the dynamics of the Potts SG model and some anticipations about the relation between precursor phenomena and thermodynamics were given. In this work we study in detail the thermodynamics of the Potts FF model, showing that T^* corresponds to the thermodynamic transition temperature T_p of the Potts variables. It is important to note that in any FF model the Griffiths temperature T_c cannot be defined for the lack of disorder. Therefore T_c cannot play any role in these cases.

Comparison of the results presented here with the analogous study of the Potts SG model with disorder [18] gives insight into the role of disorder. To this end we introduce a formal parameter $0 \leqslant X \leqslant 1$ that connects the two models. For

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$X=0$ we have the ferromagnetic Potts model [20] (without frustration and without disorder). For $0<X<1$ we have the disordered *and* frustrated Potts model. In particular, for $X=0.5$ we have the Potts SG model. For $X=1$ we have the Potts FF model (without disorder).

From Ref. [18] and from the present work, it is possible to show that for $X=0.5$ or $X=1$ there are two thermodynamic transitions. The lower transition is an Ising SG or a FF Ising transition. The upper transition at T_p is in the universality class of a ferromagnetic Potts transition. Furthermore, we show that T_p corresponds to a percolation temperature. Moreover, we show how it is possible to generalize the exact expression of T_p for the model with $X=0$ in 2D [20] to the cases $X=0.5$ and $X=1$.

The organization of the paper is as follows. In Sec. II we introduce the model and the known results for $X=0$ (ferromagnetic case), $X=0.5$ (disordered and frustrated case), and $X=1$ (ordered and frustrated case). In Sec. III we introduce the cluster formalism used to map the upper thermodynamic transition at T_p onto a percolation transition. In Sec. IV we present the phase diagram in 2D for $X=1$ as result of Monte Carlo (MC) simulations and we compare it with the cases $X=0$ and $X=0.5$. In Sec. V we use the spin-flip MC dynamics to study the dynamic critical exponent and the temperature T^*, the onset of stretched exponentials. In Sec. VI we give the summary and conclusions.

II. THE MODEL

Structural glasses, such as dense molecular glasses, plastic crystals, or ortho-therphenyl at low temperature, can be modeled to a first approximation as systems with orientational degrees of freedom frustrated by geometrical hindrance between nonspherical molecules. For this reason we will consider the lattice model introduced in Ref. [21], where the orientational degrees of freedom are represented by Potts variables [20] with s states ($\sigma_i=1,\ldots,s$) and the frustration is modeled by means of ferro/antiferromagnetically interacting Ising spins ($S_i=\pm 1$), coupled to the Potts variables.

The model is defined by the Hamiltonian

$$H_s\{S_i,\sigma_i,\epsilon_{i,j}\}=-sJ\sum_{\langle i,j\rangle}\delta_{\sigma_i,\sigma_j}(\epsilon_{i,j}S_iS_j+1), \qquad (1)$$

where the sum is extended over all the nearest neighbor sites, J is the strength of interaction, $\epsilon_{i,j}=\pm 1$ is a quenched variable that represents the sign of the ferro/antiferromagnetic interaction, and $\delta_{n,m}=0,1$ is a Kronecker delta. To emphasize that the Ising and the Potts variables are interdependent, we can rewrite the Hamiltonian in Eq. (1) as

$$H_s\{\tau_i,\epsilon_{i,j}\}=-2sJ\sum_{\langle i,j\rangle}\delta_{\epsilon_{i,j}\tau_i,\tau_j}, \qquad (2)$$

where $\tau_i\equiv S_i\sigma_i=\pm 1,\pm 2,\ldots,\pm s$ is a variables with $2s$ states and the frustration now is explicitly on the new variable. Any τ_i has an absolute value σ_i and a sign S_i.

The model depends on the interaction configuration $\{\epsilon_{i,j}\}$. Possible choices are the following. (i) If all $\epsilon_{i,j}=1$ (i.e., all interactions are ferromagnetic), Eq. (2) is the Hamiltonian of the ferromagnetic Potts model [20] with variables τ_i with an even ($2s$) number of states. It shows a thermodynamic transition at $T_c(s)$ whose order depends on s. (ii) If $\epsilon_{i,j}$ are quenched random variables, the model corresponds to the Potts SG. This model is a generalization of the Ising SG model that is recovered for $s=1$. It shows two thermodynamic transitions [18]. The lower is a SG transition at $T_{\mathrm{SG}}(s)$. The upper is a Potts transition at $T_p(s)>T_{\mathrm{SG}}(s)$. The transition at $T_p(s)$ is in the universality class of a ferromagnetic s-state Potts model. Another relevant temperature for this model is the temperature $T_c(s)$ defined for the previous case (the ferromagnetic $2s$-state Potts model). Indeed, it is possible to show that for finite external field a free energy (Griffiths) singularity arises [11]. In the limit of external field going to zero, the temperature at which this singularity occurs goes to $T_c(s)$ and the singularity vanishes. $T_c(s)$ is the Griffiths temperature for this model. Furthermore, numerical simulations [13] show that $T_c(s)>T_p(s)$ corresponds to the onset $T^*(s)$ of nonexponential correlation functions for the Ising spins S_i. This result generalizes what happens in the Ising SG ($s=1$ case), where at the Griffiths temperature $T_c(1)$ nonexponential correlation functions are seen [12]. It is worth noting that the Ising spins are critical at $T_{\mathrm{SG}}(s)$, which is well below $T_c(s)=T^*(s)$. Moreover, note that the relevant Griffiths temperature for this model is $T_c(s)$ of the variables $\tau_i=S_i\sigma_i$ and not the Griffiths temperature of the variables S_i alone, which in our notation is $T_c(1)$. (iii) If there is an odd number of $\epsilon_{i,j}=-1$ for each elementary cell (as in Fig. 1), the system is fully frustrated. This means that at least one interaction per cell is not satisfied, i.e., the relative energy contribution is 0 instead of $-2sJ$ (as for the edges *b*, *d*, and *f* in Fig. 1). The model is called a Potts FF model and is a generalization of the FF Ising model [19] which is recovered for $s=1$. It has frustration but no disorder. For any integer $s\geqslant 1$ the model has in 2D a second-order phase transition at $T=0$. Nonexponential correlation functions are reported below a finite temperature $T^*(s)$ for $s=2$, 1, and 1/2 (the last case is defined in Sec. III) [14,13]. This dynamic anomaly cannot be related, as in the previous case, to the Griffiths temperature. Indeed, the Griffiths temperature is not defined in FF models for the lack of disorder. The aim of this work is to study the phase diagram of the FF model as a function of s and to show that $T^*(s)$ corresponds

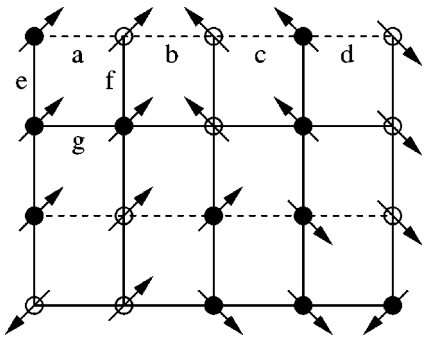

FIG. 1. Example of Potts fully frustrated model on a square lattice: on each vertex there is variable $\tau_i=S_i\sigma_i=\pm 1,\pm 2\ldots\pm s$ with $s=4$ in the figure. Here we represent the sign (S_i) of each τ_i by an open or a full circle (respectively, positive and negative, for example) and its orientational state (σ_i) by an arrow pointing in four different directions. Ferromagnetic (antiferromagnetic) interactions are represented by full (dotted) lines.

to a Potts transition. Furthermore, using a percolation approach, it is possible to show that the Potts transition corresponds to a percolation transition, defined also for noninteger values of s.

The previous three cases can be generalized to a class of Hamiltonians. Consider, as model parameter, the density X of frustrated elementary cells. For $X=0$ there are no frustrated cells (as in a ferromagnet), while for $X=1$ every cell is frustrated (FF case). For $0<X<1$ it is possible to partition the lattice into two nonoverlapping subsets $U(X)$ and $F(X)$ of unfrustrated cells and frustrated cells, respectively. Therefore Eq. (2) can be written as

$$H_{s,X}\{\tau_i\} \equiv H_s\{\tau_i, \epsilon_{i,j}(X)\} = -2sJ \sum_{\langle i,j\rangle \in U(X)} \delta_{\tau_i,\tau_j} - 2sJ \sum_{\langle i,j\rangle \in F(X)} \delta_{\epsilon_{i,j}\tau_i,\tau_j}. \quad (3)$$

In this way the ferromagnetic Potts model with an even number of states [case (i)] is recovered for $X=0$, since, $F(X=0)$ is empty; the Potts SG model [case (ii)] for $X=0.5$; the Potts FF model [case (iii)] for $X=1$, since $U(X=1)$ is empty; intermediate disordered models are obtained for other values of $0<X<1$.

To make the comparison between the $X=0.5$ and $X=1$ models, we will follow the line of Ref. [18] where the phase diagram of the former has been studied. In particular, for $X=1$ we consider a square lattice with one $\epsilon_{i,j}=-1$ per cell as shown in Fig. 1.

III. PERCOLATION

We now introduce the percolation map, following Ref. [21]. It is a generalization to $X \geqslant 0$ of Fortuin-Kasteleyn [22] cluster formalism, defined originally only for $X=0$. In Ref. [21] it is shown that the partition function $Z_{s,X}$ of the Hamiltonian in Eq. (3) can be written in terms of bond configurations C as

$$Z_{s,X} \equiv \sum_{\{\tau_i\}} e^{-H_{s,X}\{\tau_i\}/(k_B T)} = \sum_C W_{s,X}(C), \quad (4)$$

where k_B is the Boltzmann constant; $W_{s,X}(C)=0$ if C includes any *frustrated loop* (defined below) and otherwise

$$W_{s,X}(C) = p^{|C|}(1-p)^{|A|}(2s)^{N(C)} \quad (5)$$

where $p=1-\exp[-2sJ/(k_B T)]$ is the probability of placing a bond between two nearest neighbor sites [23]; $N(C)$ is the number of clusters (defined as maximal sets of connected bonds) in the configuration C; $|C|$ is the number of bonds; and $|C|+|A|$ is the total number of interactions. A loop of bonds is called *frustrated* if the product of all the signs $\epsilon_{i,j}$ of the interactions along it is equal to -1. For a frustrated loop there is no $\{\tau_i\}$ configuration able to minimize the energy of all the interactions along it. An example of such a frustrated loop is the one composed of the edges a,e,g, and f in Fig. 1 or a loop composed of the external edges of any three adjacent elementary cells in a FF lattice (or of any odd number of adjacent cells).

Note that for $X=0$ there are no frustrated loops and the original Fortuin-Kasteleyn cluster definition is recovered. Since the above cluster definition holds for any s and X, for any model described by the general Hamiltonian in Eq. (3) it is possible to define a percolation temperature for these clusters.

Moreover, the right-hand side of Eq. (4) is well defined even for noninteger values of s. In these cases it does not define a Hamiltonian model, but it still defines a percolation model. In particular, the $s=1/2$ case for $X>0$ is the *frustrated percolation* model [14].

For $X=0$, in the general case in which we consider Potts variables τ_i with a generic number q of states instead of an even $(2s)$ number of states in Eqs. (3) and (5), it is possible to show [20] that the percolation temperature $T_p(q,X=0)$ of the above defined clusters coincides with the ferromagnetic q-state Potts critical temperature $T_c(q)$. In particular, in 2D it is possible to prove [20] the relation

$$\frac{k_B T_c(q)}{qJ} = \frac{1}{\ln(1+\sqrt{q})}. \quad (6)$$

For $X=0.5$ the same kind of relation between the percolation temperature $T_p(q,X=0.5)$ and the Potts transition temperature for $q=2s$ in 2D has been obtained [18]. Furthermore, it was shown numerically that it is possible to generalize Eq. (6) using a fitting parameter $a(X)$ [18]. The resulting relation is

$$\frac{k_B T_p(q,X)}{a(X)qJ} = \frac{1}{\ln[1+\sqrt{a(X)q}]} \quad (7)$$

with $a(X=0.5)=0.800\pm0.003$ [18]. Note that $T_p(q,X=0.5)$ represents a percolation temperature for any $q \geqslant 0$ and also a Potts transition temperature for even integer values $q=2s$. Furthermore, for $0<X<1$ and $q=2s$ Eq. (6) for $T_c(2s)$ gives by definition the Griffiths temperature of the disordered model.

IV. NUMERICAL RESULTS IN 2D FOR X=1

To study the phase diagram of the model with $X=1$ (Potts FF) we have simulated it for $s=2,7,20,50$ on square FF lattices with periodic boundary conditions and linear size L from 10 to 80. At low temperature all the Potts variables tend to order ferromagnetically wherever the Ising spins satisfy the ferro/antiferromagnetic interactions (i.e., $\delta_{\epsilon_{i,j}S_i,S_j}=1$). In particular, at $T=0$ the system in 2D has a second-order phase transition of the Ising spins, as in the FF Ising model [19]. We will show that the interplay between Potts variables and Ising spins affects the phase diagram at finite temperature. As in Ref. [18], to study the finite temperature range we can use an efficient cluster dynamics with an annealing procedure. We define a MC step as an update of the whole system. At each temperature we average the data over 10^4 MC steps, discarding the first 5×10^3 MC steps.

In our systematic analysis we calculated for each s the

Binder parameter [24] for the energy density E defined as

$$V=1-\frac{\langle E^4\rangle}{3\langle E^2\rangle^2} \tag{8}$$

(angular brackets denote the thermal average). This quantity allows us to distinguish between first-order and second-order phase transitions. Indeed, in a second-order phase transition for $L\to\infty$ it is $V=2/3$ for all temperatures, while in a first-order phase transition V has a well pronounced minimum near the transition temperature. The thermodynamic of the model is studied by means of the Potts order parameter

$$M=\frac{s\max_i(M_i)-1}{s-1} \tag{9}$$

(where $i=1,\ldots s$, M_i is the density of Potts spins in the ith state), the susceptibility

$$\chi=\frac{1}{k_BT}\frac{\langle M^2\rangle-\langle M\rangle^2}{N} \tag{10}$$

(where N is the total number of Potts spins), and the specific heat

$$C_H=\frac{1}{k_BT^2}\frac{\langle E^2\rangle-\langle E\rangle^2}{N}. \tag{11}$$

To study the Fortuin-Kasteleyn percolation we calculated the percolation probability per spin $P=1-m_1$ and the mean cluster size $S=m_2$ (where $m_n=\Sigma_k k^n n_k$ is the nth moment of the distribution of density n_k of clusters with size k).

A. The second-order transition for s=2

For $X=1$ and $s=2$ the Binder parameter V goes to the constant value 2/3 for all temperatures as L increases (see Fig. 2) revealing a second-order phase transition. The transition temperature T_s in the thermodynamic limit can be estimated, together with all the critical exponents, using the standard scaling analysis [25] for second-order phase transitions. By definition of the critical exponents ν, β, γ, and α, it is $\xi\sim|T-T_s|^{-\nu}$, ξ being the correlation length, $M\sim|T-T_s|^{\beta}\sim\xi^{-\beta/\nu}$, $\chi\sim|T-T_s|^{-\gamma}\sim\xi^{\gamma/\nu}$, $C_H\sim|T-T_s|^{-\alpha}\sim\xi^{\alpha/\nu}$, for which we expect

$$M\sim L^{-\beta/\nu}f_M((T-T_s)L^{1/\nu}) \tag{12}$$

(and analogous scaling laws for χ and C_H) where $f_M(x)$ is a universal function of the dimensionless variable x. The values at which the scaling laws are satisfied give estimates of the critical exponents and of T_s. In Fig. 3 we show the large-size data collapse using the set of Ising critical exponents [26] and leaving only T_s as a free parameter, giving an estimate $k_BT_s/J=2.73\pm0.03$.

Study of the percolation quantities shows a smooth behavior of P and a cusp in S increasing with L. Therefore one can make the ansatz that the percolation transition is of second order. Let us define a Fortuin-Kasteleyn percolation temperature T_p and a set of percolation critical exponents ν_p, β_p, and γ_p by means of the relations $\xi_p\sim|T-T_p|^{-\nu_p}$, where ξ_p is the connectedness length of the clusters (i.e., the typical linear cluster size) and $P\sim|T-T_p|^{\beta_p}\sim\xi_p^{-\beta_p/\nu_p}$, $S\sim|T-T_p|^{-\gamma_p}\sim\xi_p^{\gamma_p/\nu_p}$. Applying the standard scaling analysis for percolation [27], one obtains in a consistent way the results summarized in Fig. 4 using the corresponding thermodynamic critical exponents for the 2D Ising model. The numerical estimate for the percolation temperature is $k_BT_p/J=2.73\pm0.03$, coincident with the estimates of T_s. Therefore the percolation transition and the Potts transition occur at the same temperature and with the same set of critical exponents, i.e., they coincide.

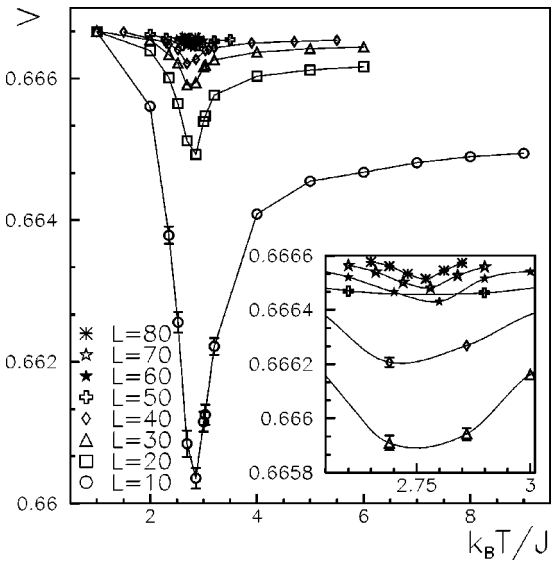

FIG. 2. $X=1$ and $s=2$: Binder's parameter V vs T for the lattice sizes L listed in the figure. Inset: Enlarged view. Where not shown, errors are smaller than symbol size. Lines are only guides for the eyes. For increasing L, V goes to 2/3 for all temperatures, showing a second-order phase transition.

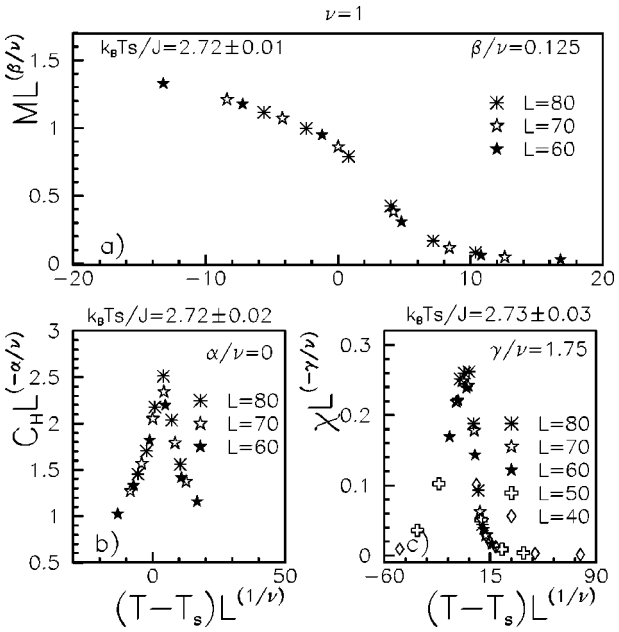

FIG. 3. $X=1$ and $s=2$: Collapse of M, C_H, and χ data in (a), (b), and (c), respectively, for the Ising critical exponents $(\nu,\beta,\alpha,\gamma)$. Each collapse gives an independent estimate of the critical temperature T_s (indicated in each panel).

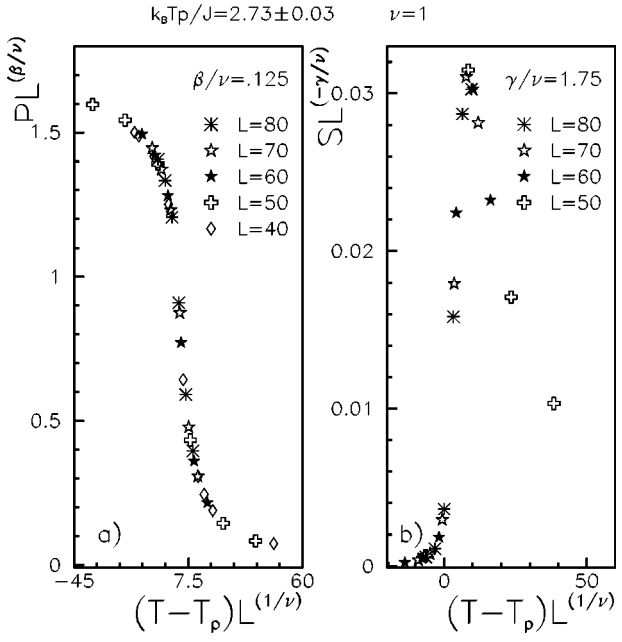

FIG. 4. $X=1$ and $s=2$: Collapse of P and S data in (a) and (b), respectively, for the Ising critical exponents. Each collapse gives an estimate of the percolation temperature $k_B T_p/J=2.73\pm0.03$.

B. The first-order transition for s=7, 20, and 50

For $X=1$ and $s=7$, 20, and 50 we have considered systems with L from 10 to 50 lattice steps with periodic boundary conditions. On the base of the mean field results [17] for the Potts FF model and the knowledge of the Potts model [20], we expect that the order of the transition will change for $s>4$. In fact, the thermodynamic order parameter M becomes more and more discontinuous as s increases. At the same time the percolation order parameter P develops a more and more pronounced discontinuity.

In particular, study of the Binder parameter V reveals that the model for $s=7$, 20, and 50 has a first-order phase transition, since, for each considered lattice size L between 10 and 50, V has a nonvanishing minimum, as shown in Fig. 5 for $s=7$. In these cases the estimates of infinite-size transition temperatures $T_s(s)$ and $T_p(s)$ for the thermodynamic and percolation transition, respectively, can be made through the relation [25]

$$T_{\max}(L)-T_{\max}(\infty)\sim L^{-D}, \tag{13}$$

where $D=2$ is the Euclidean dimension, $T_{\max}(L)$ is the finite-size temperature of the maximum of C_H or S, and $T_{\max}(\infty)$ is the transition temperature in the thermodynamic limit. Therefore $T_s(s)$ and $T_p(s)$ can be evaluated by linear fits on a log-log scale with one free parameter. The results are summarized in Table. I. For any s, $T_s(s)$ and $T_p(s)$ are consistent within the numerical error.

TABLE I. $X=1$ and $s=7,20,50$: Numerical estimates of thermodynamic transition temperature $T_s(s)$ and percolation transition temperature $T_p(s)$. For any s they are consistent within the numerical error.

s	T_s	T_p
7	6.87 ± 0.04	6.85 ± 0.06
20	15.3 ± 0.1	15.3 ± 0.1
50	31.7 ± 0.1	31.5 ± 0.1

C. Phase diagram

The numerical results in Secs. IV A and IV B give rise to the phase diagram for $X=1$. It is qualitatively similar to the phase diagram for $X=0.5$ [18]. In Fig. 6 we compare both of them with the phase diagrams for $X=0$.

For $X=0$ (Potts model with $2s$ state variables) for any integer s there is a paramagnetic/ferromagnetic phase transition at finite temperature $T_c(s)$. The transition is of second order for $2s\leqslant4$ and of first order for $2s>4$ [20]. $T_c(s)$ is given by Eq. (6) with $q=2s$. It coincides with the Fortuin-

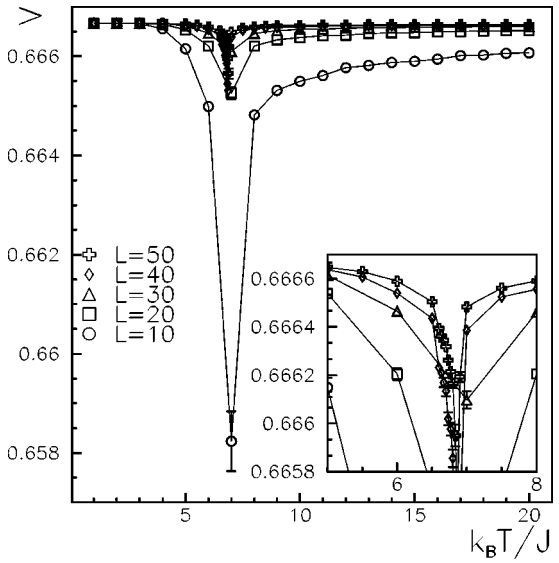

FIG. 5. $X=1$ and $s=7$: Binder's parameter V as in Fig. 2. V has a well defined minimum for any size, showing a first-order phase transition.

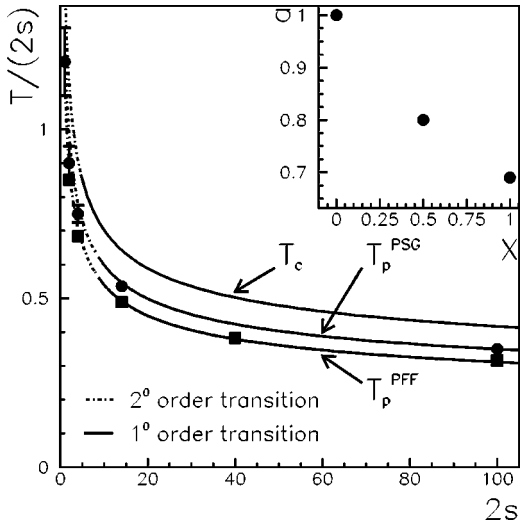

FIG. 6. Numerical phase diagram in 2D for $X=0$ (Potts model: T_c), $X=0.5$ (Potts SG model: T_p^{PSG}) and $X=1$ (Potts FF model: T_p^{PFF}). The data are fitted with Eq. (7) with fit parameter $a(X)$ shown in the inset. Errors are smaller than symbol size.

Kasteleyn percolation temperature. The percolation temperature is defined even for noninteger values of s.

For $X=0.5$ (Potts SG model with frustration induced by disorder and with $2s$ state variables) there are two phase transitions for integer values of s. The lower transition is a SG transition. It is assumed to occur at $T_{SG}=0$ for any s in 2D and at $T_{SG}(s)>0$ in higher dimensions as in the Ising SG [28]. The high-temperature transition is an s state Potts ferromagnetic transition occurring at $T_p(s,X)$ given by Eq. (7) with $q=2s$ and $a(X=0.5)=0.800\pm0.003$ [18]. It is a second-order transition for $s\leqslant 4$ and a first-order transition for $s>4$. $T_p(s,X)$ corresponds also to the Fortuin-Kasteleyn percolation temperature, which is defined even for noninteger s [18]. This model is disordered and its Griffiths temperature is by definition the transition temperature of the $2s$ state Potts model $T_c(s)$, given by Eq. (6) with $q=2s$. It is possible to see that $T_c(s)$ is numerically consistent with the onset of nonexponential relaxations at $T=T^*(s)$ for $s=2$ in 2D [13] and for $s=1$ (Ising SG) in 2D and 3D [12,29].

For $X=1$ (Potts FF model with frustration and no disorder and with $2s$ state variables) considered here, there are two transitions for integer values of s, as well as for $X=0.5$. The lower transition is at $T_{FF}=0$ in 2D and at $T_{FF}(s)>0$ in higher dimensions, as for the FF Ising model ($s=1$) [19,32]. As seen in this section, in this case the upper transition is an s state Potts ferromagnetic transition at $T_p(s,X=1)$. As shown in Fig. 6, Eq. (7) describes $T_p(s,X=1)$ well, using a fit parameter $a(X=1)=0.690\pm0.003$. Furthermore we have shown that it coincides with a Fortuin-Kasteleyn percolation transition. As a consequence the Fortuin-Kasteleyn clusters represent the regions of correlated Potts variables. This means that the cluster's characteristic linear size is equal to the correlation length of the Potts variables. Analyses for $s=1/2$ (frustrated percolation) and $s=1$ (FF Ising model) in 2D and 3D are given in Ref. [14].

The main difference between the $X=1$ and $X=0.5$ cases is that the Griffiths temperature is defined in the latter (disordered model), but not in the former (for the lack of disorder). The important consequence of this fact is that for $X=1$ the dynamic anomalies are present only below $T_p(s,X=1)$ [30], while for $X=0.5$ they are present also above $T_p(s,X=0.5)$ and below $T_c(s)$ [31].

Note that all the Potts percolation transition temperatures for $X=0$, 0.5, and 1 can be described by the same form in Eq. (7) as a function of s with an X-dependent parameter $a(X)$. This parameter has a regular behavior as function of X (see the inset in Fig. 6).

V. DYNAMIC CRITICAL EXPONENT

As shown in Sec. IV A, at $T_p(s=2,X=1)$ the Potts variables have a second-order phase transition. Therefore their correlation length diverges and their dynamics slows down. A measure of the slowing down for any observable A is given by the dynamic critical exponent z defined by $\tau_A(T_p(L),L)\sim L^z$. Here, omitting for the sake of simplicity the dependence on s and X, $T_p(L)$ is the transition temperature for the system with finite size L [33] and $\tau_A(T,L)$ is the correlation time at temperature T and size L associated with the correlation function for A,

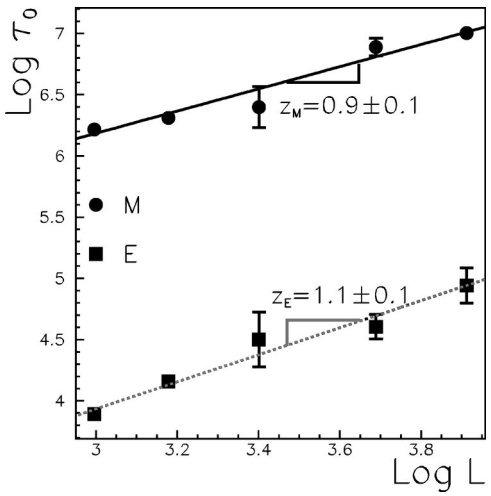

FIG. 7. $X=1$ and $s=2$: The logarithm of correlation time τ_0 (see text) at the finite-size transition temperature $T_p(L)$ [33] as function of the logarithm (base 10) of size L, for the correlation function of the Potts order parameter M (circles) and of the energy density E (squares), for $L=20,24,30,40$, and 50. The slopes give the exponents z_M and z_E.

$$f_A(t,T)=\frac{\langle A(t,T)A(0,T)\rangle-\langle A(T)\rangle^2}{\langle A(0,T)^2\rangle-\langle A(T)\rangle^2}, \tag{14}$$

where t is the time. More then one definition of τ_A is possible for any A, but all of them, even if numerically different, have the same qualitative behavior [12]. In particular, facing the difficulty that the greater the size, the greater $\tau_A(T_p(L),L)$, we define τ_M and τ_E for the Potts order parameter M and the energy density E as the time τ_0 (in units of MC steps) at which $f_M(\tau_0,T_p(L))=0.4$ and $f_E(\tau_0,T_p(L))=0.3$, respectively. The data for sizes $L=20$, 24, 30, 40, 50 are shown in Fig. 7 and the dynamic critical exponents are estimated by linear fits on a log-log plot as $z_M=0.9\pm0.1$ and $z_E=1.1\pm0.1$ [34].

To study the behavior of f_M and f_E in the thermodynamic limit we have extrapolated the data in the infinite-size limit following the procedure suggested in Ref. [36]. It consists in plotting at any t the generic $f_A(t,T,L)$ for finite-size L versus $1/L$ and in extrapolating for $1/L\to 0$. We consider the temperature range $2.65<k_BT/J<3.25$ [35]. The results are shown in Figs. 8 and 9. To check the form of f_M and f_E, we have fitted the data with three different plausible functions: (a) a simple exponential $f_0\exp(-t/\tau)$; (b) a Kolraush-Williams-Watts stretched exponential $f_0\exp[-(t/\tau)^\beta]$; (c) the Ogielski form

$$f(t,T)=f_0\frac{e^{-(t/\tau)^\beta}}{t^x}, \tag{15}$$

which is a combination of form (b) with a power law. In the previous functions, f_0, τ, x, and β are T-dependent parameters. Note that for the form (c) it is possible to estimate f_0 and x separately from β and τ, since the first two describe the short-time behavior and the second two the long-time regime.

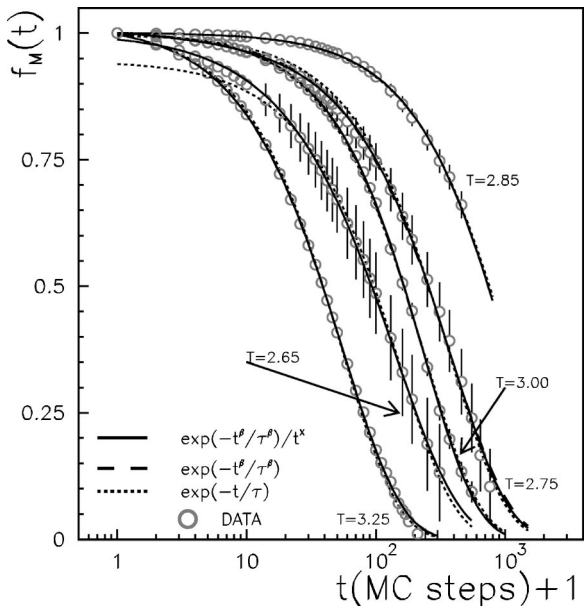

FIG. 8. $X=1$ and $s=2$: Correlation function of the Potts order parameter M in the thermodynamic limit (see text). For clarity we show only some of the recorded data for the simulated temperatures. Symbols are results of simulations, solid lines are fits with the form in Eq. (15), dashed lines (on this scale indistinguishable from solid lines) with stretched exponential form and dotted lines with exponential form. Where not shown, the errors are smaller than the symbol size. Temperature is measured in J/k_B.

The Ogielski form turns out to describe f_M and f_E very well as shown in Figs. 8 and 9. The fitting parameters are presented in Fig. 9 and 10. The forms (b) and (c) always give compatible estimates of the β exponent, consistent with the very low values of x (which is approximately the slope of the function at $t=0$ in Figs. 8 and 9).

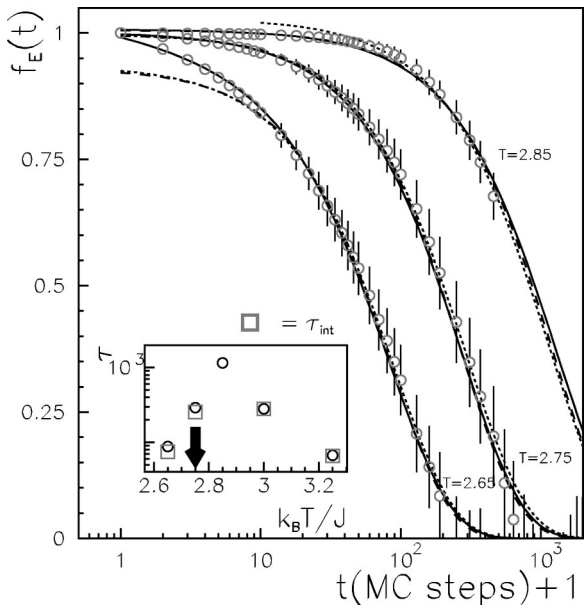

FIG. 9. $X=1$ and $s=2$: Correlation function of the energy density E in the thermodynamic limit as in Fig. 8. Inset: The correlation times estimated by exponential fit (circles) and by Eq. (16) (squares). The arrow shows the numerical estimate of T_p.

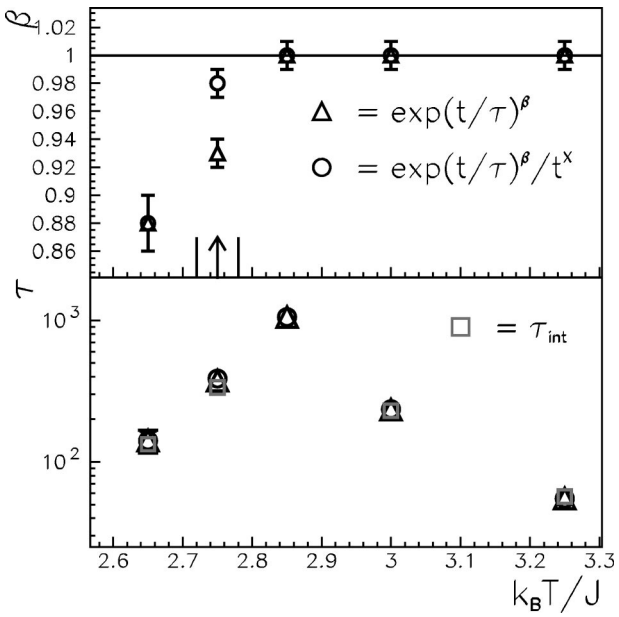

FIG. 10. $X=1$ and $s=2$: Fit parameters for f_M data with form as in Eq. (15) (circles) and for stretched exponential form (triangles). In the lower panel we show also the integral correlation times τ_{int} estimated with Eq. (16) (squares). The arrow and the vertical lines show T_p and the numerical indeterminacy on it, respectively.

From Fig. 10 for the parameter β of f_M, we see that it is $\beta=1$ above the Potts transition at $k_BT_p/J=2.73\pm0.03$ and $\beta<1$ below T_p. Therefore there is a dynamic transition between a high-temperature exponential behavior and a low-temperature stretched exponential behavior of f_M. This result shows the presence of a complex dynamics below T_p, consistent with analysis of the nonlinear susceptibility correlation function of the Ising spins [13]. It is important to note that, while the Potts variables have a transition at T_p, the Ising spins have no transition at T_p and, in principle, no dynamical anomalies are expected for them.

On the other hand, the data for f_E show that the long-time behavior is well described by an exponential function. In particular, the form (c) with $\beta=1$ and a nonzero x fits very well also the data for the lowest temperature considered here. Note that, in principle, one can expect a dynamical anomaly even for the energy density E, since it depends explicitly on the critical Potts variables.

In the fitting forms used, the correlation time τ is defined as a fitting parameter. Another possible definition is the following (integral correlation time):

$$\tau_{int,A}(T)=\lim_{t_{max}\to\infty}\frac{1}{2}+\sum_{t=0}^{t_{max}} f_A(t,T). \tag{16}$$

Due to the divergence of the correlation time, the definition in Eq. (16) does not converge near the transition temperature. Therefore it is not shown in Figs. 9 and 10 for the temperature with the largest τ. However, where it converges, all the different estimates of the correlation time are numerically consistent as shown in Figs. 9 and 10. Note that, even if the data are extrapolated to the thermodynamic limit, finite-size effects are still present. Indeed, the critical temperature esti-

mated from τ measurements, within our temperature mesh, is between $2.75J/k_B$ and $2.85J/k_B$, which is at variance with the estimate of T_p.

VI. SUMMARY AND CONCLUSIONS

We have studied a schematic model for glasses where frustrated orientational degrees of freedom, associated with $2s$ state Potts variables τ_i, induce complex dynamics. In real systems the frustration can be associated, for example, with steric hindrance of nonspherical molecules in structural glasses. Each τ_i has an absolute value ($\sigma_i=1,\ldots,s$) and a sign ($S_i=\pm 1$). The frustration is over the signs and can be *with* disorder or *without* disorder, depending on a model parameter X. For $0<X<1$ there is disorder, while for $X=1$ the model is (fully) frustrated without disorder. For $X=0$ there is no frustration, and the model recovers the $2s$ state ferromagnetic Potts model.

For $0<X\leqslant 1$ the model has two thermodynamic transitions. The high-temperature transition at $T_p(s,X)$ for the model with $2s$ states is in the universality class of the s-state ferromagnetic Potts model. Therefore the fluctuations (χ and C_H) of the orientational degrees of freedom diverge at $T_p(s,X)$ (for $s\leqslant 4$), as well as the correlation times of quantities depending on them (like the Potts order parameter M or the energy density E). For them we estimated the dynamic critical exponents z_M and z_E. The low-temperature transition is a spin glass transition for $X=0.5$, or a fully frustrated transition for $X=1$, and marks the ordering transition of the signs S_i (Ising variables).

The diverging fluctuations at the upper and lower transition temperatures are expected to be experimentally observable only using specific probes that couple with them. Examples of such probes could be those associated with dielectric measurements in supercooled liquids and plastic glassy crystals or with electron spin resonance spectroscopy measurements [6,7].

For $X=1$ and $s=2$ the model shows a complex dynamics corresponding to T_p. In particular, the correlation function for M and the correlation function for the signs S_i change their behaviors. They have an exponential behavior above T_p and a nonexponential behavior below T_p. This behavior is expected at least for any $s\leqslant 4$, because it is associated with the free energy singularity occurring at the second-order transition of the Potts variables. Therefore the complex dynamics corresponds to a real thermodynamic transition.

For $X=0.5$ and $s=2$ the onset of this dynamic anomaly is shifted to a higher temperature, *above* T_p. It occurs in correspondence with the Griffiths essential singularity of the free energy. This singularity is not defined in the $X=1$ case. For zero external field it goes to the transition temperature of the ferromagnetic $2s$-state Potts model $T_c(2s)$ and vanishes. Therefore the onset of complex behavior does not correspond to a real thermodynamic transition.

We have shown that the Potts transition at $T_p(s,X)$ for any s and X considered here coincides with a percolation transition. It is not worthless to note that the dynamic transition at $T_p(s,X=1)$ persists also for $s=1$ and $s=1/2$ [14]. In these cases $T_p(s,X=1)$ does not correspond to a thermodynamic transition, but only to a percolation transition. Therefore for $s<2$ the dynamic anomaly is no longer related to a thermodynamic transition, but to a percolation transition in real space [14]. This result could be related to experimental results on microemulsions [8].

Finally, we have shown that it is possible to generalize the exact relation for the ferromagnetic Potts transition temperature $T_c(s)$ in 2D to a transition temperature $T_p(s,X)$ for any $0\leqslant X\leqslant 1$, using a fitting parameter $a(X)$. In particular, $a(X)$ acts like a renormalization factor for the number of states of the model; it is $a(X=0)=1$ (ferromagnetic case) and $a(X)$ decreasing regularly with increasing X.

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