The Potts frustrated model: relations with glasses

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ABSTRACT

Similarities between fragile glasses and spin glasses (SGs) suggest the study of the frustrated spin model in order to understand the complex dynamics of glasses above the glass transition. We consider a frustrated spin model with Ising spins and s-state Potts spins both with and without disorder. We study the two models by Monte Carlo simulations in two dimensions. The Potts spins mimic orientational degrees of freedom, and the coupled frustrated Ising spins take frustration into account, such as the geometrical hindrance. We show that in this model dynamical transitions and cross-overs are related to static transitions. In particular, when disorder is present, as predicted and verified in SGs, a dynamical transition between high-temperatures exponential to low-temperatures non-exponential correlation functions numerically coincides with the ordering temperature of the ferromagnetic regions, that is the Griffiths temperature $T_{c(s)}$, while a cross-over between power-law growth of correlation times to Arrhenius law occurs near a Potts transition at $T_{p(s)} < T_{c(s)}$. In the model without disorder, where $T_{c(s)}$ is not defined, both the dynamical transition and the cross-over occur at $T_{p(s)}$. Furthermore the static susceptibility and the autocorrelation times of quantities depending on the Potts spins diverge at $T_{p(s)}$. This is reminiscent of recent experimental results on glass-forming liquids.

§ 1. INTRODUCTION

Glassy systems, like supercooled liquids, polymers, granular material, vortex glasses, ionic conductors, colloids, plastic crystal and spin glasses (SGs), can be defined as materials characterized by a slowing down of one or more degrees of freedom which prevents the system from reaching equilibrium as the temperature decreases (Angell 1984, 1995, Götte 1989, Ediger et al. 1996).

In particular, SGs are dilute alloys of magnetic atoms in a low concentration in a non-magnetic matrix where the relevant degrees of freedom are the impurity spins interacting via random magnetic couplings. The randomness gives rise to frustration, that is competition that prevents the systems from minimizing the global free energy (Mézard et al. 1987).

One of the characteristic phenomena of glassy systems is their complex dynamics well above the calorimetric glass transition at temperature $T_g$. For example there is a dynamical transition at $T^* > T_g$ from high-temperature exponential to low-temperatures non-exponential correlation functions. Another feature is the cross-over at $T_1$
with $T_g < T_1 < T^*$ between a high-temperature power-law growth of correlation times to an Arrhenius behaviour $\tau = \exp(\Delta E/k_B T)$, where $\Delta E$ is the activation energy. This phenomenology is well seen in experiments (Angell 1984, 1995, Ediger et al. 1996 Andreozzi et al. 1998).

Here we show the numerical results on frustrated models with and without disorder, the Potts spin-glass (PSG) and the Potts fully frustrated (PFF) model respectively, where the dynamical anomalies correspond to static transitions, giving some insight into the relation between dynamics and statics in glassy systems and clarifying the role played by frustration and by disorder. The model could also be useful in understanding some recent experimental results on finite-temperature diverging static susceptibility in glassy systems (for example Dixon et al. (1990), Menon and Nagel (1995) and Leheny and Nagel (1997)).

§ 2. THE POTTS SPIN-Glass AND POTTs FULLY FRUSTRATED MODELS

Let us consider the Hamiltonian

$$H = -sJ \sum_{i,j} \left[ \delta_{\sigma_i \sigma_j} (\epsilon_{i,j} S_i S_j + 1) - 2 \right],$$

where with each lattice site is associated an Ising spin $S_i = \pm 1$ and an $s$-state Potts spin $\sigma_i = 1, \ldots, s$. The sum is extended over all nearest-neighbour (NN) sites, $\epsilon_{i,j} = \pm 1$ is the sign of interaction and $J$ is the strength of interaction. When the $\epsilon_{i,j}$ are quenched random variables, we shall refer to the model as the PSG model, while, when they are distributed in a deterministic way to frustrate each lattice cell, we shall refer to it as the PFF model. For $s = 1$ the PSG (PFF) model recovers the Ising SG (fully frustrated (FF)) model.

The model can be interpreted as a system with $s$-state orientational degrees of freedom frustrated by means of coupled Ising spins which take into account effects due to geometrical hindrance (e.g. as in plastic crystals, where the centres of mass of the molecules form a regular crystal but the molecules are frustrated with respect to the orientational degrees of freedom, or in o-terphenyl or in glycerol). The way in which the frustration is introduced distinguishes this model from other models, for example the Potts glass model (Kirkpatrick and Wolynes 1987, Thirumalai and Kirkpatrick 1998), used to study structural glasses.

Both the PSG and the PFF models can be mapped on a Fortuin–Kasteleyn (FK) (1972) percolation model (Coniglio and Klein 1980), defining the FK clusters as maximal sets of spins connected by bonds activated between NN spins with probability $p - 1 - \exp(-2sJ/k_B T)$ ($k_B$ is the Boltzmann constant) when both the NN Potts and the Ising spins minimize the coupling energy and using the relation

$$Z_s(C) = \sum_{W_s(C)} \exp \left( -\frac{H}{k_B T} \right) \prod_{i,j} W_s(C),$$

where $W_s(C) = 0$ if the cluster configuration $C$ contains any frustrated loop (defined below); otherwise $W_s(C) = p^{|C|} (1 - p)^{|A|} (2s)^{|N(C)|}$ where $N(C)$ is the number of clusters in the configuration $C$, $|C|$ is the number of activated bonds and $|A|$ is the total number of interactions. A frustrated loop is a closed path that has an odd number of antiferromagnetic interactions (Coniglio et al. 1991). While the Hamiltonian (1) is defined only for integer $s > 1$, the partition function (2) is meaningful for any value of $s$ (Fierro et al. 1999).
§ 3. Statics and dynamics of the models

The numerical phase diagrams of the PSG and PFF model have been given by Franzese and Coniglio (1998) and Franzese (1999) and are qualitatively reproduced in figure 1 for the three-dimensional case. Two transition temperatures are seen. The lower temperature \( T_{SG}(s) \) (or \( T_{FF}(s) \)) corresponds to a SG (or FF respectively) transition in the universality class of \( \pm J \) Ising SG (or Ising FF) model. The higher \( T_{P}(s) \) corresponds to the percolation transition of FK clusters and for any integer \( s > 1 \) marks a real thermodynamic transition in the universality class of a ferromagnetic \( s \)-state Potts model (Wu 1982). At \( T_{P}(s) \) the susceptibility of Potts spins diverges (Franzese and Coniglio 1998, Franzese 1999). In the PSG model, above \( T_{P}(s) \), there is the Griffiths temperature \( T_{c}(s) \) defined as the critical temperature of a ferromagnetic model with the same number of states of the disordered model (2s for the s-state PSG model). This transition is a consequence of the presence of ferromagnetic regions, due to disorder, and vanishes for vanishing external field (Griffiths 1969).

From the dynamical point of view we have studied (Franzese 1999, Franzese and Coniglio 1999) for \( s = 2 \) both for the PSG model and the PFF model the time-dependent nonlinear susceptibility

\[
\chi_{SG}(t) = \frac{1}{N} \left( \sum_{i} S_i(t + t_0) S_i(t_0) \right)^2
\]  

(where \( N \) is the total number of spins and \( t_0 \) is the equilibrium time) that converges asymptotically for \( t \rightarrow \infty \) to the usual static nonlinear susceptibility. The normalized correlation function is

\[
f_x = \frac{\chi_{SG}(t) - \chi_{SG}(t \rightarrow \infty)}{\chi_{SG}(0) - \chi_{SG}(t \rightarrow \infty)},
\]

with \( \chi_{SG}(0) = N \). Following Campbell and Bernardi (1994) the infinite size behaviour of \( f(t) \) has been extrapolated at every \( t \) plotting the data for finite linear sizes \( L = 20, 25, 30 \) and \( 40 \) against \( 1/L \).

![Figure 1. Qualitative phase diagram for the PSG model in three-dimensions as function of \( s \): (-----) real thermodynamic phase transitions; (---), vanishing Griffiths transition; (X), Potts vanishing transition in the \( s = 1 \) (\( \pm J \) Ising SG) case. An analogous phase diagram holds for the PFF model with a FF Ising phase at the place of the SG phase and without the G phase.](image_url)
To test the form of $f(t)$ we fitted the data as follows:

(i) with a simple exponential, finding good fits only asymptotically for long times and for high temperatures;

(ii) with a stretched exponential function $f_0 \exp\left(\left(t/\tau\right)^\beta\right)$, finding that it fails to fit the data only for short times;

(iii) with the form $f_0 t^{-x} \exp\left(\left(t/\tau\right)^\beta\right)$ suggested by Ogielski (1985), finding that it fits very well the data over all the time range and the temperature range (Franzese and Coniglio 1999).

The parameters $\beta$ and $\tau$ used in the fits (ii) and (iii) for $\chi_{SG}$ are plotted in figures 2 and 3 for the PSG model and the PFF model respectively. In the same figures is shown also the integral correlation time defined as

$$\tau_{int} = \lim_{t_{max} \to \infty} \left( \frac{1}{2} \int_{t=0}^{t_{max}} f(t) \, dt \right), \quad (5)$$

where $f$ is the generic correlation function.

In figure 2 for the PSG model it is possible to distinguish three dynamical regions: a high-temperature region for $T > T^* \approx T_c(s)$ where the correlation functions are exponential ($\beta = 1$); an intermediate region for $T^* > T > T_1 \approx T_P(s)$ where $\beta < 1$ and the correlation time growth is consistent with a power law forecast by the mode coupling theory (MCT) (Götze 1989) or mean-field (MF) theory (for example Bouchaud et al. (1998) and references therein); a lower-temperature region
for $T < T_1$ where activated processes dominate the dynamics (i.e. the correlation times follow an Arrhenius law) as in the experimental glasses (Angell 1984, 1995, Ediger et al. 1996, Andreozzi et al. 1998). These results show that the prediction $T^* - T_c$ given for the SG (Randeria et al. 1986, Cesi et al. 1997) is valid also in this model.

In figure 3 for the PFF model, where $T_c(s)$ is not defined in the absence of disorder, the intermediate region disappears and both the dynamical transition at $T^*$ and the cross-over at $T_1$ occur at a temperature numerically consistent with $T_p(s)$.

For the PFF model we have calculated also the correlation functions for the Potts order parameter $M = \langle |M_i - 1|/(s-1) \rangle$ (where $M_i$ is the density of Potts spins in the $i$th state) defined as

$$f_M(t) = \frac{\langle \delta(t + t_0) \delta(t_0) \rangle}{\langle \delta(t_0)^2 \rangle},$$

(6)

(where $\delta(t) = M_i(t) - \langle M_i \rangle$ and $t_0$ is the equilibration time). At the Potts transition temperature $T_p(s)$ the static susceptibility related to $M$ diverges (Franzese 1999) and the parameter $\beta$ and $\tau$ for fit (ii) and (iii) of $f_M$ becomes less than one and diverging respectively, as shown in figure 4. The divergence of $\tau$ is obtained from the observation that $\tau(T,L)$ grows for increasing $L$ at any $T$ and there is a cusp at a temperature consistent to $T_p(s)$ within numerical error.

§ 4. Conclusions

The PSG model and the PFF model reproduce the experimental phenomenology of fragile glasses above the glass transition, recovering the dynamical transition between the exponential and non-exponential correlation functions and the crossover
between a non-Arrhenius growth, predicted by the MF and MCT theories, and the activated Arrhenius regime for the correlation times. In particular, the disordered PSG model shows three different dynamical regimes experimentally seen for spin-$\frac{1}{2}$ probes in glass-forming liquids such as o-terphenyl (Andreozzi et al. 1998).

The models show that these dynamical transitions and cross-overs can be related to static thermodynamic transitions: in the PSG model to the Griffiths transition and to the Potts transition, while in the PFF model only to the Potts transition. The mapping of these models on the FK percolation model show that the Potts transition coincides with a percolation transition where frustrated loop are excluded, giving a geometrical interpretation of the effects of frustration.

Furthermore at the Potts transition the susceptibility associated with the Potts variables diverges. This result is reminiscent of recent experimental findings (for example Dixon et al. (1990), Menon and Nagel (1995) and Leheny and Nagel (1997)). In the models presented here this divergence is explained by the ordering of the orientational degrees of freedom. Whether such a divergence is present also in structural glasses such as plastic crystals is matter of debate (Schneider et al. 1999).

Moreover the PFF model emphasizes that dynamical anomalies are not related to the presence of frustration and disorder, but also to the sole frustration; in this case $T_P$, that is the ordering temperature of the orientational degrees of freedom, marks the onset of these anomalies. This could be relevant in the study of dynamical behaviour of experimental FF systems such as Josephson junction arrays.

**References**


