Finite-size scaling at the dynamical transition of the mean-field 10-state Potts glass

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Abstract

We use Monte Carlo simulations to study the static and dynamical properties of a Potts glass with infinite range Gaussian distributed exchange interactions for a broad range of temperature and system size up to $N = 2560$ spins. The results are compatible with a critical divergence of the relaxation time $\tau$ at the theoretically predicted dynamical transition temperature $T_D$, $\tau \propto (T - T_D)^{-\Delta}$ with $\Delta \approx 2$. For finite $N$ a further power law at $T = T_D$ is found, $\tau(T = T_D) \propto N^{z_*}$ with $z_* \approx 1.5$ and for $T > T_D$ dynamical finite-size scaling seems to hold. The order parameter distribution $P(q)$ is qualitatively compatible with the scenario of a first order glass transition as predicted from one-step replica symmetry breaking schemes.

29. September, 2000
PACS numbers: 64.70.pf, 75.10.Nr, 75.40.Gb

Developing a theory of the glass transition of a fluid from its Hamiltonian within first principles statistical mechanics is still a formidable problem [1,4]. While some researchers attribute glassy freezing to the (hypothetical) vanishing of the configurational entropy $\mathcal{F}$ at the “Kauzmann temperature” $T_K$ (which is lower than the experimental glass transition temperature $T_g$), others emphasize the dynamical transition at the critical temperature $T_c$ of mode coupling-theory from the ergodic fluid to a non ergodic state. Since, for atomic systems, $T_c > T_g$, this frozen phase can have only a finite lifetime and is thought to decay by thermally activated (so-called “hopping”) processes.

Recently evidence has been given [3,4] that these two seemingly different scenarios could both result as two complementary aspects of the same unifying theory [7]. In view of the questions that still exist on the various theoretical approaches, it is valuable to have exactly solvable models that exhibit a similar behavior: a dynamical transition at a temperature $T_D$ and a static first order glass transition at a temperature $T_0 < T_D$. One of these models is the $p$-state infinite range Potts glass with $p > 4$ [8,13], where at $T_0$ a static (Edwards-Anderson type) spin glass order parameter $q_{EA}$ appears discontinuously. However at $T_0$ there is neither a latent heat nor a divergence of the static spin glass susceptibility $\chi_{SG}$. The latter would diverge only at an extrapolated spinodal temperature $T_s < T_0$, see Fig. 1. The dynamical behavior of the spin autocorrelation function $C(t)$ for $T \gtrsim T_D$ is described by the same type of equations [12,13] as found in mode-coupling theory [2]. Thus this model seems indeed to have many properties in common with structural glasses. Apart from being a possible prototype model for the structural glass transition, the Potts glass can also be
considered as a simplified model for an anisotropic orientational glass: e.g. a six-state Potts glass may be a reasonable description of a diluted cubic molecular crystal where diatomic molecules can align only along the \( p = 6 \) face diagonals \[16\].

In order to understand this model in more detail, we have performed extensive Monte Carlo simulations. Of course these simulations were done for systems with finite size and thus all the transitions in Fig. 1 are rounded. While in the past finite size effects at normal first and second order transitions have been studied extensively \[17,18\], very little is known about finite size effects at dynamical transitions. Thus it is hoped that the present work will be useful for the proper analysis of simulations of realistic models for the structural glass transition as well \[19\]. In addition, finite mean-field systems may also have some similarities with systems having finite interaction range \[20\]: the relaxation time \( \tau \) is large but finite for \( T < T_D \) as well, unlike the behavior in the thermodynamic limit \( N \to \infty \) (shown in Fig. 1), since energy barriers between “basins” are finite for \( T < T_D \) \[20\]. Thus the mean field Potts glass for finite \( N \) should be a good model for elucidating the physics of glassy systems in general.

We now give some technical details about our simulations. We study the Hamiltonian

\[
H = -\frac{1}{2} \sum_{i \neq j}^N J_{ij}(p\delta_{\sigma_i\sigma_j} - 1),
\]

where each spin \( \sigma_i \in \{1, \ldots, p\} \) interacts with all the other spins. The interactions \( J_{ij} \) are taken from a Gaussian distribution with mean \( J_0 = (3 - p)/(N - 1) \) and variance \( \Delta J = (N - 1)^{-1/2} \). We choose \( p = 10 \) (note that for \( p = 2 \) the standard Ising spin glass results \[15\]). For this choice of \( \Delta J \) it can be shown \[4\] that \( T_s = 1 \) \[21\]. We simulate the system sizes \( N=160, 320, 640, 1280 \) and \( 2560 \), and the number of independent samples is \( 500 \) for \( N=160 \) and \( T > 1 \), else \( 100 \), with the exception of \( N=2560 \) where only \( 50 \) samples were used. The equilibrium dynamics is studied by means of the standard Metropolis algorithm \[15–17\]. In order to produce equilibrated configurations and to study the static properties we used again the Metropolis algorithm at high temperature \( (T \leq T_D) \), while for lower temperatures we used the parallel tempering method \[22,23\].

Fig. 2 shows typical data for the autocorrelation function \( C(t) \) of the Potts spins \[24\] at two temperatures and various system sizes. While at very high temperature, such as \( T = 1.8 \), finite size effects are completely negligible, at \( T = T_D \) they are unexpectedly pronounced. Whereas in the thermodynamic limit one expects at the dynamical transition \( C(t \to \infty) = q_{EA} \), for \( N \lesssim 1280 \) hardly any indication of the development of the plateau (as expected from Fig. 1) is seen. This behavior is strikingly different from the behavior found in analogous autocorrelation functions for atomistic models of structural glasses, where a pronounced plateau occurs already at temperatures a few percent above \( T_c \) (= \( T_D \) in our model) \[13\] and finite size effects are hardly detectable for a comparable range of \( N \). While for \( N \to \infty \) the dynamics of the present model for \( T > T_D \) is described by mode-coupling theory \[12,13\], the assertion that infinite range models for finite \( N \) resemble the behavior of real structural glasses \[20\] seems, in view of Fig. 2, doubtful to us, at least for the system sizes presently accessible.

In order to quantify the slowing down of the dynamics as a function of the temperature and system size we define a relaxation time \( \tau \) by \( C(\tau) = 0.2 \). This particular choice was made since we must have \( C(\tau) < q_{EA}(T = T_D) \). Our results indicate that, for \( T = T_D \), \( \tau \)
behaves like a power law $\tau \propto N^{z^*}$ with $z^* \approx 1.5$ (see inset in Fig. 3). It is known from the analytical results [13] that, in the limit $N \to \infty$, $\tau(T) \propto (T/T_D - 1)^{-\Delta}$. The dynamical finite size scaling hypothesis [17,18,25] assumes a generalized behavior for $\tau$ as a function of $N$ and $T$ for $T \gg T_D$,

$$\tau = N^{z^*} \tilde{\tau}\{N(T/T_D - 1)^{\Delta/z^*}\} \text{ for } N \to \infty \text{ and } (T/T_D - 1) \to 0 \quad (2)$$

with the scaling function $\tilde{\tau}(\xi \to \infty) \propto \xi^{-z^*}$ to recover the proper thermodynamic limit. As can be seen from our data in Fig. 3, this ansatz is satisfied by the Potts glass in the vicinity of the dynamical transition. Our choice of $\Delta/z^* \approx 1.3$ in Fig. 3 implies $\Delta \approx 2$, which is similar to values found for atomistic models of the glass transition [19] and compatible with a direct extrapolation $N \to \infty$ of the data for $\tau(T, N)$ for $T > T_D$ [26].

We mention that Eq. (2) has a well-based theoretical foundation for second order phase transitions [15,24], where in Fig. 1 $T_0 = T_D = T_s$ would coincide. However, for a dynamical transition which has no associated diverging static susceptibility this relation is purely phenomenological. For second order mean-field spin glass transitions one has Eq. (2) with $\Delta/z^* = 2\beta_{MF} + \gamma_{MF} = 3$, where $\beta_{MF} = 1, \gamma_{MF} = 1$ are the static mean-field exponents of the spin glass order parameter and the susceptibility, respectively [27]. Since $\Delta = 2$ [13] one has $z^* = 2/3$, consistent with expectation [28] and simulations [24]. Obviously, in view of the systematic deviations from scaling that are still visible in Fig. 3, our estimates for $\Delta$ and $z^*$ clearly are somewhat tentative only.

We conclude by discussing some results about some static properties of this model. As usual in numerical simulations of spin glasses, the order parameter is a measure of the overlap between microscopic states visited by two different replicas (same realization of disorder, but different dynamics) of the system. For Ising spin glasses, this is just the number of spins in the same state divided by the total number of spins. In the Potts glass, as well as in vector and quadrupolar spin glasses, the overlap between spins belonging to different replicas is a tensorial quantity. Therefore we define an overlap order parameter which is invariant under global rotations of the spins [13,16]:

$$q_{\alpha\beta} = \sqrt{\sum_{\mu,\nu=1}^{p-1} (q^{\mu\nu})^2} \quad \text{with} \quad q^{\mu\nu} = \frac{1}{N} \sum_i S^\mu_{i,\alpha} S^\nu_{i,\beta},$$

where $\alpha$ and $\beta$ are the replica indices and $S^\mu_{i,\alpha}$ are the components of the spins in the simplex representation [24]. The static spin glass susceptibility is defined as $\chi_{SG} = N[\langle q_{00}^2 \rangle]$. Our Monte Carlo results (Fig. 4) are indeed compatible with the expected behavior for static quantities: the spin glass susceptibility remains finite at $T = T_D$ and the order parameter distribution $P(q)$ develops a two peak structure not by splitting off a single peak when the temperature is lowered, as would be common for second-order transitions [13,18]. Instead the second peak grows near $q = q_{EA}$ continuously gaining weight for low temperatures. This temperature dependence is consistent with a one-step replica symmetry-breaking scenario [12].

In summary we have shown that the finite size rounding of the dynamical transition in the $p = 10$ infinite range Potts glass is compatible with a finite size scaling hypothesis, and that the relaxation time at the dynamical transition scales like a power law, $\tau \propto N^{z^*}$, with $z^* \approx 1.5$. The static spin glass susceptibility converges to a finite results at $T_D$, as expected.
In contrast to atomistic models for the glass transitions, this model allows well equilibrated simulations at $T = T_D$ and also much lower temperatures (Fig. 4), at least for $N$ in the range of a few hundreds. While atomistic models allow to study questions such as the dynamical heterogeneity only at $T > T_D$ (which would not be a relevant temperature region in this context for experiments), the present model allows to determine the relaxation behavior of various quantities over a much wider temperature range. Hence from the present model we expect that a rather complete picture of the glass transition can be obtained, which thus should give stimulating insights into the proper analysis of simulations for more realistic models too, and help in clarifying the fundamental questions that still remain about the nature of glassy freezing in structural glasses.

Acknowledgments: One of us (C.B.) was partially supported by the Deutsche Forschungsgemeinschaft, Sonderforschungsbereich 262/D1. We are grateful to the John von Neumann Institute for Computing (NIC Jülich) for a generous grant of computer time at the CRAY-T3E.
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[24] $C(t) = 1/N \sum_{i=1}^{N} \langle \langle \vec{S}_i(t') \cdot \vec{S}_i(t'+t) \rangle \rangle$, where $[\cdots]$ is the sample average, and the thermal average $\langle \cdots \rangle$ is an average over the initial time $t'$. As usual, we use here the simplex representation where the $p$ states $\sigma$ correspond to $(p-1)$-dimensional unit vectors $\vec{S}$ pointing towards the corners of a $p$-simplex, see F. Y. Wu, Rev. Mod. Phys. 54, 235 (1982). Thus $C(t=0) = 1$ and $C(t \to \infty) = 0$.
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The standard mean-field result for critical relaxation in spin glasses with short-range forces is $\tau \propto L^z$ with a dynamical exponent $z = 4$, where $L$ is the linear dimension of the system. This result can be translated into the behavior of infinite range models at the marginal dimension $d^*$ where mean-field theory becomes valid, $d^* = 6$, via $N = L^{d^*}$, i.e. $z^* = z/d^* = 2/3$. 

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FIG. 1. Qualitative sketch of the mean-field predictions for the $p$-state Potts glass model with $p > 4$. The spin glass order parameter in thermal equilibrium is positive only for $T < T_0$ and jumps to zero discontinuously at $T = T_0$, where the spin glass susceptibility $\chi_{SG}$ is finite (for $T > T_0$, $\chi_{SG}$ follows a Curie-Weiss type relation with an apparent divergence at $T_s < T_0$). The relaxation time diverges already at the dynamical transition temperature $T_D$. This divergence is due to the occurrence of a long lived plateau in the time-dependent spin autocorrelation function $C(t)$.

FIG. 2. Spin-spin autocorrelation function $C(t)$ for $T = 1.8$ and for $T = T_D = 1.142$ \[1\], for several values of $N$. The solid line is the theoretical value of the Edward-Anderson order parameter $q_{EA}(T_D)$ for $N \to \infty$ \[1\]. The dashed line locates the value we use to define the relaxation time $\tau$. 
FIG. 3. Log-log plot of the scaled relaxation time $\tau/N^{z^*}$ vs. the scaled distance in temperature $N(T/T_D - 1)^{\Delta/z^*}$ from the dynamical transition temperature, choosing $z^* = 1.5, \Delta/z^* \approx 1.3$. The inset is a log-log plot of $\tau(T = T_D)$ vs. $N$.

FIG. 4. Inverse of the spin glass susceptibility $\chi_{SG}^{-1}$ plotted vs. $T^{-2}$. Different symbols correspond to different values of $N$. The number of different samples used is 300 for $N = 160$, 200 for $N = 320$ and 100 for $N = 640$ and 1280. Arrows locate $T_s, T_0, T_D$ [11]. The inset shows the order parameter distribution $P(q)$ vs. $q$ for $N = 320$ and various temperatures.