The High Temperature Dynamics of a mean field Potts glass

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We use Monte Carlo simulations to investigate the dynamical properties of the infinite range 10 states Potts glass. By analyzing the spin autocorrelation function for system sizes up to $N = 2560$, we show that strong finite size effects are present around the predicted dynamical transition temperature. The autocorrelation function shows strong self-averaging at high temperatures, whereas close to the dynamical transition they show the lack of self-averaging.

1 Introduction

In recent years a new class of disordered spin glass models has been introduced (for a review see Kirkpatrick and Thirumalai 1995) that show strong analogies with the theoretical scenario proposed for the structural glass transition, such as the presence of a dynamical transition at a temperature $T_D$ and a static phase transition (with discontinuous order parameter but without latent heat) at $T_0 < T_D$. Furthermore, the equations of motion for the spin autocorrelation functions are formally analogous to the equations of motion of the density-autocorrelation functions introduced by the mode coupling theory of the glass transition (Götze 1989). One example of such spin models is the $p$ states mean field Potts glass with $p > 4$ (Kirkpatrick and Wolynes 1987, Kirkpatrick and Thirumalai 1988). The goal of the present paper is to compare the relaxation dynamics of such a system with a finite size with the dynamics of the system in the thermodynamic limit. The latter has previously been determined at the level of one step replica symmetry breaking (De Santis et al. 1995). Furthermore we investigate to what extend the time correlation functions are self-averaging or not.

2 Model and Simulations

In the Potts model each spin $\sigma_i$ is a discrete variable that can take one of $p$ different values: $\sigma_i \in \{1, \ldots, p\}$. The Hamiltonian is given by

$$H = - \sum_{i,j} J_{ij} (p \delta_{\sigma_i \sigma_j} - 1),$$

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i.e. each spin interacts with all the others. The coupling constants $J_{ij}$ are taken from a Gaussian distribution

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi(\Delta J)}} \exp \left[ -\frac{(J_{ij} - J_0)^2}{2(\Delta J)^2} \right].$$

(2)

We consider the case $p = 10$ since for this case the static transition has a strong first order character (jump of the order parameter from zero to $q_0 = 0.452$) (De Santis et al. 1995). Note that for $p = 2$ we recover the Sherrington-Kirkpatrick model. It has been shown that in order to prevent the system from ordering ferromagnetically, a negative value of $J_0$ has to be chosen (Elderfield and Sherrington 1983, Gross et al. 1985, Cwilich and Kirkpatrick 1989) and therefore we have chosen $J_0 = (3 - p)/(N - 1)$. The variance is set to $\Delta J = (N - 1)^{-1/2}$ and in the following we will set the Boltzmann’s constant $k_b = 1$. With these units a numerical solution of the replica equations at the level of one step replica symmetry breaking predicts a dynamical transition at $T_D = 1.142$ and a static transition from a paramagnet to a spin glass at $T_0 = 1.131$ (De Santis et al. 1995).

We have simulated 5 different system sizes, $N = 160, 320, 640, 1280$ and 2560 spins, at various temperatures. In this paper we will focus on temperatures between $T = 1.8$ to $T_D = 1.142$, i.e. the range above the dynamical transition temperature in the thermodynamic limit. Due to the random nature of the interactions, we have to average all observables not only over the canonical distribution but also over the possible realizations of the disorder given by Eq. (2). In the following we will denote this latter average by $\cdot$. For this we used 500 different samples for 160 spins, 100 for 320, 640 and 1280 spins and between 20 and 50 for 2560 spins. The dynamics is generated using the Metropolis algorithm. Starting from a given spin configuration, a spin is picked at random and assigned a new random orientation. If the energy difference between these two states is negative the move is accepted. If it is positive it is accepted only with probability $\exp (-\Delta E/T)$.

3 Results

We present now our results regarding the analysis of the spin-spin autocorrelation function, defined as

$$C(t) = \frac{p}{p - 1} \frac{1}{N} \sum_{i}^{N} \left[ \langle \delta_{\sigma_i(v')\sigma_i(v+t)} - 1/p \rangle \right].$$

(3)

The mean field theory predicts that in the thermodynamic limit the dynamics of the system slows down upon approach of the (dynamical) transition temperature $T_D$. The relaxation time $\tau(T)$ for the time correlation function should show at $T_D$ a divergence of the form $\tau \propto (T - T_D)^{-\Delta}$. At the same time the spin autocorrelation function is predicted to show at intermediate times a plateau with a height $q_{EA} = 0.328$ before it decays on the time scale $\tau$ towards zero. At $T = T_D$ the system becomes nonergodic in that the correlation function does not show anymore the final decay, i.e. it stays at the plateau even for infinite times. (For a review of this
behavior on a class of spin glass systems see Thirumalai and Kirkpatrick 1995. For the works regarding the Potts glass, see Kirkpatrick and Wolynes, 1987 and Kirkpatrick and Thirumalai, 1988).

However, for a finite system we do no longer expect the sharp ergodic to nonergodic transition at $T_D$, since for $N < \infty$ the relaxation times have to remain finite for all $T > 0$. It is therefore of interest to see how the typical relaxation behavior of the system changes if $N$ is increased.

In Fig. 1 we show the temperature dependence of $C(t)$ for 1280 spins. From the figure we see that with decreasing temperature the dynamics does indeed slow down. However, even at $T_0 < T_D$ we do not see a pronounced sign for the existence of the dynamic transition, since the curves show, instead of the expected plateau at $q_{E_A}$ (shown in the figure as solid horizontal line), only a weak shoulder. Thus we conclude that the dynamics of this system is strongly affected by finite size effects even for systems as large as 1280 spins. The reason for this is that the barriers in the free energy that separate one “basin” of configuration space from a neighboring “basin” are apparently not very high, in contrast to the thermodynamics limit in which their height diverges. Note that this $N$ dependence of the dynamics is in marked contrast with the one found in structural glasses since in these systems finite size effects are usually absent if the system has more than a few hundred particles (Kob 1999).

To study in more detail how the relaxation dynamics depends on the size of the system we show in Fig. 2 the time correlation function for different system sizes for a high temperature, and at $T = T_D$. At the high temperature the different $C(t)$ fall nicely onto a master curve, i.e. there are no finite size effects. This is in stark contrast to the behavior at $T_D$. At this temperature we find that the relaxation dynamics for the different system sizes depends strongly on $N$ since the large systems relax much slower than the small ones. If one defines a relaxation time $\tau(T)$ via $C(\tau) = 0.2$, see horizontal dashed line in the figure, one finds that, at $T_D$, these times show a power-law dependence: $\tau \propto N^{1.5}$ (Brangian et al. 2001). Note that the value of 1.5 for the exponent is significantly larger than the estimate $2/3$ for the Sherrington-Kirkpatrick model (Bhatt and Young 1992).

Using a dynamical finite size scaling Ansatz we have found that in the thermodynamic limit we expect a divergence of the relaxation time of the form $\tau \propto (T - T_D)^{-2}$ (Brangian et al. 2001). Thus the exponent $-2$ is close to the values found for structural glasses (Götze 1999).

In the remaining of this paper we will concentrate on the self-averaging properties of $C(t)$. Knowing these properties will help to decide whether or not it is necessary to average the results of a simulation over many independent realizations of the disorder even in the case that the size of the system is very large. Suppose that we have determined the thermal average $X_i$ of an observable $X$. (Here $i$ stands for the realization of the disorder.) Following Wiseman and Domany (1998, and references therein) we consider the quantity $R_X$ defined as follows:

$$R_X = \frac{[X_i^2] - [X_i]^2}{[X_i]^2}. \tag{4}$$

Here $[\cdot]$ stands again for the average over the disorder. Usually one has the situation of “strong self averaging” which means that $R_X \propto 1/N$ for $N \gg 1$. The case
$R_X \propto 1/N^\alpha$, with $\alpha < 1$ is denoted by “weak self averaging”. Finally the case $R_X = \text{const.}$ is called “non self-averaging”.

In Fig. 3 we show the spin autocorrelation function for system size $N = 1280$ and for 20 representative samples. From the figure it becomes clear that at high temperatures the sample to sample fluctuations are quite small and that therefore the system is probably self-averaging. For a temperature close to $T_D$ this is, however, not the case in that the fluctuations are now on the same order as the typical relaxation time.

To study this effect in a more quantitative way we use the relaxation time $\tau$ as the observable $X$ discussed above. Using thus equation (4) to define the quantity $R_\tau$ we can investigate the $N$ dependence of $R_\tau$. In Fig. 4 we show the temperature dependence of $R_\tau N$ for all system sizes investigated (main figure), with error bars that have been determined with the jackknife method (Newman and Barkema 1999). We see that for high temperatures we do indeed find that this quantity goes to a constant of order one, independent of the system size. Hence we conclude that $R_\tau$ is proportional to $1/N$ and that hence the system is strong self-averaging. At low temperatures this is, however, no longer the case since there we see that the product increases with increasing system size and becomes, for the largest systems, as large $O(10^3)$. Thus this is evidence that the system is no longer self-averaging. To investigate this point closer, we plot in the inset $R_\tau$ at $T_D$ as a function of $N$. (Note that at this temperature we do not have data for the largest system size since the relaxation time becomes too large.) From this graph we see that the value of $R_\tau$ is basically constant within the noise of the data, or shows even a slight trend to increase. Thus this is evidence that at this temperature the system is not self-averaging. We also mention that we expect that for sufficiently large $N$ self-averaging will be recovered for all $T > T_D$, although our data are not conclusive on this issue for $T \leq 1.3$, due to the strong finite size effects.

To conclude, we have analyzed the dynamics of a 10 states infinite range Potts glass. Analytical results show that that this is a spin model which resembles in many points structural glasses. We have shown that the mean field scenario can, from a qualitative point of view, also be seen in systems with finite $N$. However, close to the transition temperature dynamical as well as static quantities are strongly affected by finite size effects. In particular we find that the dynamics of the system shows a crossover from a self-averaging behavior to a non self-averaging behavior as the temperature approaches $T_D$.

**Acknowledgements:** C.B. was partially supported by the Deutsche Forschungsgemeinschaft, Sonderforschungsbereich 262/D1. W.K. and K.B. are grateful to the German Israeli foundation (GIF) for travel support. We thank the RUS for a generous grant of computing time on the Cray T3E.
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Figure 1: Spin autocorrelation function $C(t)$ versus $t$ (measured in units of Monte Carlo steps per spin) for 1280 spins at various temperatures. The horizontal solid line shows the position of the Edward Anderson order parameter in the thermodynamic limit.

Figure 2: Spin autocorrelation functions for different system sizes at two different temperatures, $T = 1.8$ and $T = 1.142 = T_D$. The horizontal solid line shows the position of the Edward Anderson order parameter in the thermodynamic limit. The dashed line is used to define the relaxation time $\tau(T)$.
Figure 3: Correlation functions for different realization of disorder. System with 1280 spins, temperature $T = 1.5$ and $T = 1.142 = T_D$

Figure 4: Plot for the scaled quantity $R_X \cdot N$ as a function of temperature; the inset shows $R_X$ as a function of the system size at $T = 1.142 = T_D$