Crystal vs Glass Formation in Lattice Models with Many Coexisting Ordered Phases

Mário J. de Oliveira, Alberto Petri, Tânia Tomé

Abstract

We present here new evidence that after a quench the planar Potts model on the square lattice relaxes towards a glassy state if the number of states \( q \) is larger than four. By extrapolating the finite size data we compute the average energy of these states for the infinite system with periodic boundary conditions, and find that it is comparable with that previously found using fixed boundary conditions. We also report preliminary results on the behaviour of these states in the presence of thermal fluctuations.

Key words: Lattice models, glasses, non-equilibrium phenomena

PACS: 05.50.+q, 61.43.Fs, 64.60.-i

1 Introduction

A variety of lattice models has been devised in the last years in order to account for the freezing of liquids into a disordered state rather than ordering into their crystalline forms after a sudden cooling below the solidification temperature. Most of these models are based on a certain amount of quenched disorder which prevents them from ordering [1]. Others are provided of dynamical [2] constrains aimed to the same purpose. These models have been proven very useful for discovering and understanding many important features of the disordered systems. However they cannot reveal the mechanisms that prevent crystallisation in systems with ordered ground states.

Very recently departure from crystallisation has been observed even in some models which do not possess any of the above ingredients and that on the
contrary have crystalline ground states [3]. Strong metastability, typical of
the transition from liquid to glass, has been first observed in a model of Ising
spins on a cubic lattice [4,5] where the product of the four spins of each
plaquette contributes to the total energy with a same coupling constant (4-
spin, or FSIM model). The model, which at equilibrium shows a first order
transition, also displays stretched exponential relaxation and aging properties
at low temperatures [6].

An interesting question concerns the origin of this behaviour and its relation-
ship with models that relax into ordered ground states. In some recent works
[7,8,9] we have investigated the quench of two kinds of simple models on the
square lattice, i.e. exclusion models and Potts model, and found that under
appropriate circumstances also these models may relax to glassy rather than
to crystalline or polycrystalline phases. The glassy phase is distinct from the
polycrystalline phase in that the length of the line separating different do-
mains is of the order of the number of sites in the system, thus being different
from the usual coexistence of different phases at thermodynamic equilibrium.
The behaviour is determined by the number $q$ of (equivalent) ground states
that the system possesses: in both kinds of models a glassy phase is attained
for $q > q_c$, whereas polycrystalline states are attained for $2 < q < q_c$. A re-
markable point is that this change from ordering to glassiness in the relaxation
process, corresponds to the change from second to first order transition in the
considering equilibrium diagram, which occurs at the same $q_c$ for both kind
of systems.

The onset of a glassy phase is not in contradiction with thermodynamics,
according to which the system evolves towards a uniform phases. In fact it is
obtained under the prescription of taking the thermodynamic ($L \to \infty$) limit
before the ergodic ($t \to \infty$) limit. Thermodynamics would require the ergodic
limit to be taken before the thermodynamic limit.
Here we present some new findings. The next section reports some results on the Potts model with different $q$ when subject to a quench at $T = 0$ with periodic boundary conditions (PBC). Section three deals with the onset and the stability of the glassy phase at finite temperature, and all results are summarised in section four.

2 Periodic boundary conditions at $T = 0$

The Potts model with $q$ states may be defined by the Hamiltonian:

$$H = \sum_{ij} (1 - \delta_{s_i, s_j}),$$

where the sum is on nearest neighbour pairs, $s_i$ is the state variable of the site $i$ which can assume the values $1, 2, \ldots, q$, and $\delta_{a,b}$ is the Kronecker’s function.

It is known since a long time that after a quench from high temperature to $T = 0$ the system relaxation slows down and eventually stops when single spin dynamics is employed. This is due to the formation of locally stable configurations, like the one shown in Fig.1, which in the absence of thermal fluctuations, keep the system’s dynamics pinned. To overcome the problem of finite size effects, in our previous work [7,8,9] the quench was performed by imposing fixed boundary conditions (FBC), thus forcing the system to finally fall into one of its ordered ground states. The glassy phase was then predicted by the increase of the relaxation time with the system size and the length of the line separating the different domains was obtained by a suitable extrapolation to $L = \infty$ and $t = \infty$.

| $q$ | PBC | FBC |
|-----|-----|-----|
| 3   | 0.00| 0.000|
| 5   | 0.07| 0.060|
| 7   | 0.11| 0.105|

Table 1

Blocked configurations observed with PBC have energies that, besides to depend on the system size, fluctuate strongly from one realization to the other. Maybe for these reasons they have been generally considered some kind of finite size artifact and, to our knowledge, they have never been investigated in a systematic way. We have performed several quenches of the Potts model on square lattices with increasing size $L$, using PBC and different values of $q$. For
Fig. 2. Average energy reached by the system after a quench from $T = \infty$ to $T = 0$ as a function of the system linear size $L$. Curves for $q = 5$ and $q = 7$ display a tendency to saturate, not shown by the curve for $q = 3$. Each $L$, the average energy per site $u$ of the blocked configurations obtained is reported in Fig.2, together with its statistical fluctuation, for $q = 3, 5$ and 7. While it shows to approach an asymptotic value for $q = 3$, this does not seem the case for $q = 5$ and 7.

In order to attempt quantitative predictions the same quantity has been plotted on a different scale in Fig.3. The horizontal scale is chosen in such a way to make the lines as straight as possible. This happens by choosing $1/\sqrt{L}$ as plotting variable, but we have no theoretical argument for this choice. Extrapolation to $L = \infty$ yields the average energy $u^*$ expected for the blocked configurations in the thermodynamic limit. A comparison of these values with those obtained by using FBC [7,8,9] is reported in Table 1 and confirms our previous conclusions, that is for $q > 4$ the quench leads to a glassy phase: the length of the line separating different domains contribute with an energy which does not vanish in the limit of infinite system. We did not investigate the case $q = 4$ which is critical [7,8,9] and might require logarithmic corrections.

3 Stability against thermal fluctuations

Our previous work [7,8,9] concerned the behaviour of Potts and exclusion model after a quench at $T = 0$ [10]. Here we report some preliminary results on two different cases. The first is the case in which the quench is performed at a low but finite temperature. The energy decay of the Potts model with $q = 7$ after a quench at $T = 0.1$, is plotted in Fig.4 for different system size as a function of the expected domain size. As this latter increases, two main trends may be singled out: i) the relaxation to the ground state (forced by
Fig. 3. The limit energy per site $u^*$ displayed in Fig. 2 appears to behave linearly when plotted as function of $1/\sqrt{L}$. Extrapolation to $L = \infty$ yields values compatible with those obtained when using FBC, reported in Table I.

Fig. 4. The relaxation to equilibrium after a quench from $T = \infty$ to $T = 0.1$. Relaxation to the ground state takes place later and the energy decreases less, when the system size increases.

the use of FBC) takes places at later times; ii) it starts at increasing values of the energy. Although yet preliminary, these evidences indicate that the system would relax to a state with finite energy even when quenched at a temperature that is about 0.13 of the critical temperature. More work in this direction is still needed for drawing quantitative conclusions.

The second case concerns the investigation of the time taken by the system to escape from a metastable configuration because of thermal fluctuations. The system is initially at $T = \infty$; then it is quenched to $T = 0$ and left to relax into a metastable state. This is numerically checked by verifying that
Fig. 5. Distribution of the logarithm of escape times from a metastable state, for the Potts model with $q = 7$, when the temperature is raised from $T = 0$ to $T = 0.4$. In the inset it is plotted the typical time. Note the log scale on the time axis.

the system energy cannot decrease further by changing state to a single site. Then temperature is raised again to a finite values $T_e$, and the time needed to overcome the energy barrier is computed as the time needed to reach the thermal equilibrium energy corresponding to that temperature.

Figure 5 reports the time distribution for $q = 7$ and $T_e = 0.4$, which is more than half the critical temperature. Histograms are computed over 10,000 realizations for $L = 16$ and 32, and on more than 1000 realizations for $L = 64$. Owing to the large statistics required, only results for small systems are available at present, more work being in progress. The data show that the distribution of the logarithm of escape times is approximately Gaussian, but a distortion towards large times seems to develop for $L = 64$. It should be noted that the number of quenches leading to states with the energy of the ground state vanishes and that the typical escape time, shown in the inset, grows about exponentially when the system size increases. It is expected to be proportional to the height of the free energy barriers separating metastable phases by stable ones. In the Potts model this height grows as $\exp(L^{d-1})$ [11].

4 Summary

We have reported here some recent results on the onset of glassy states after the quench of the Potts model on a square lattice. By a method different from previous work, they confirm that these states occur when the number of ground states $q$ is larger than four [7,8,9]. By extrapolating the computed average energies we found values for the infinite system that are compatible with those found with the previous method for the three values of $q$ investigated.
Preliminary results show that the glassy state is attained also by quenching at small but finite $T$, and that for $q = 7$ the time needed by the system to exit from a local energy minimum by thermal fluctuations seems to increase exponentially with the system size for temperatures of the order of half the critical temperature.

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