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CONICET

Relaxational dynamics of the q-state Potts model

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ABSTRACT

We investigated the relaxation towards equilibrium of the q-state Potts model in a square lattice after a cooling with rate r (including $r\to\infty$, i.e. quenching) from an equilibrium state at $T>T_c$ to different target temperatures in the range $0<T<T_c$, being T_c the critical temperature. We worked mainly in the $q=9$ Potts model with periodic boundary conditions, using numerical simulations with both standard Monte Carlo (MC) method (Glauber dynamics) and continuous time MC or *n-fold* technique [1]. The latter allowed us to extend our simulations to a wide range of time scales. We analyzed the behavior of the average energy as a function of time. We also calculated the probability distribution of the *relaxation-time* needed to reach the equilibrium state. The observation of instantaneous spin configurations (snapshots) during individual realizations of the system relaxation helped us to identify the different domain growth mechanisms involved. We observed the existence of different dynamical regimes, according to the quench temperature range, namely:

i. For temperatures smaller but very close to T_c we found evidence of a super-cooled disordered meta-stable state, in agreement with one of the two possible scenarios proposed by K. Binder [2]; relaxation in this case is dominated by nucleation of the stable phase.
ii. For lower target temperatures, but still not very close to zero, our numerical data are consistent with a *normal* coarsening process, obeying an Allen-Cahn law, namely $l(t)\sim t^{1/2}$, being $l(t)$ the average domain size.
iii. For temperatures close to zero we found evidences of a partially disordered, slow decaying non-equilibrium state; such state has been previously reported for smaller values of q [3-6] and exhibit several characteristics of glassy systems.

In both (ii) and (iii) regimes we observed that, for large system sizes, the system sometimes *gets trapped* at later stages of the relaxation in some particular, highly symmetric configurations, that we called *blocked-states.* This happens in a non-negligible percentage of the realizations. The relaxation from the blocked states occurs through an activated mechanism, where the size of the associated barriers appears to be independent of the system size for large values of N. We identified two different types of blocked states: macroscopic ferromagnetic stripes parallel to the lattice coordinates and macroscopic hexagonal-shaped ferromagnetic domains. While the former have been previously observed in the two dimensional Ising model ($q=2$) [7], the latter (as far as we know) has not been previously reported and is in agreement with early theoretical predictions of Lifshitz [8] for large values of q.

The Potts Model:

We study the 9-state Potts model in a two-dimensional square lattice L × L , with periodic boundary conditions.

The Hamiltonian of the model can be written as:

$$H=-J\sum_{\langle i,j\rangle}\delta(\sigma_i,\sigma_j)\quad,\ \sigma=1,2,\ldots 9\quad,\quad \delta(\sigma,\sigma')=\begin{cases}1 & \text{if } \sigma=\sigma'\\ 0 & \text{if } \sigma\neq\sigma'\end{cases}$$

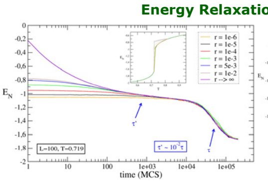
The internal energy of the system is defined as: $E=\langle H\rangle$

For q ≥ 4 this model is known to exhibit a first-order phase transition at [9] :

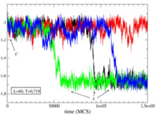
$$\frac{k_B T_c}{J}=\left[\ln(1+\sqrt{q})\right]^{-1}$$

and a continuous transition for q<4. For q=9 we have a strong first-order transition at T_c=0,7213 well defined, we assume K_B = J = 1.

Energy Relaxation



Energy per spin relaxation for a 100x100 lattice after coolings with different rates r


The system jumps at a stochastic time τ from the super-cooled state to the steady state.

We define the non-linear relaxation energy function as [2] :

$$\phi_E(t)=\frac{E(t)-E(\infty)}{E(0)-E(\infty)}$$

E(∞) ≡ <E> is the stable state energy

We propose the following two states model:

$$\phi_E(t,\tau)=\phi_{E1}\,\Theta(\tau-t)+\phi_{E2}(1-\Theta(\tau-t))$$

$\Theta(x)$ is the Heaviside step function

We assume a distribution:

$$P(\tau)=\frac{1}{\tau\sigma\sqrt{2\pi}}\exp\left(-\frac{(\ln(\tau)-\mu)^2}{2\sigma^2}\right)\qquad,\ \tau>0$$

For the stochastic nucleation time τ, and calculates it's mean value as:

$$\langle\phi_E(t)\rangle=\int_0^\infty P(\tau)\,\phi_E(t,\tau)\,d\tau$$

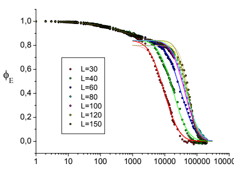
obtaining:

$$\langle\phi_E(t)\rangle=\phi_{E1}-\frac{(\phi_{E1}-\phi_{E2})}{2}\,\mathrm{erfc}\left(\frac{\mu-\ln(t)}{\sqrt{2}\,\sigma}\right)\qquad(*)$$

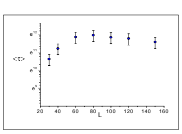
where *erfc(x)* is the complementary error function . Then

$$\langle\tau\rangle=\exp(\mu+\sigma^2/2)$$

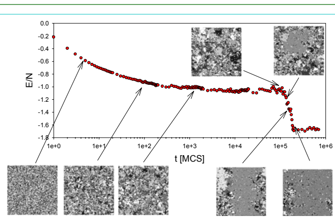
We fit (*) to our simulations for different lattice sizes, imposing ϕ_{E2}= 0 and ϕ_{E1} and letting free the parameters μ and σ. The error bars for <τ> where obtained varying ϕ_{E1} around the plateau's ϕ_E value.



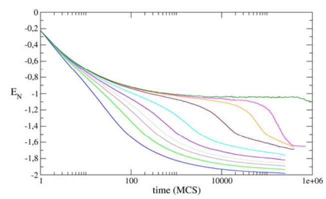
Relaxation energy function for a 100x100 sistem after a cooling with $r=10^{-4}$ to T=0,719.


<τ> scaling with L

These results are in agreement with the those postulated by the Classic Nucleation Theory [10].

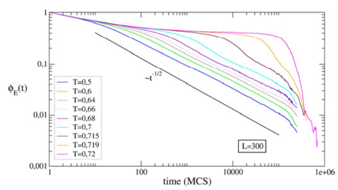


Typical escape from the metastable state: energy relaxation and snapshots of the lattice at different times for a N=150x150 system at T=0,72, different grey shades represent different magnetic phases (q possible for each spin).



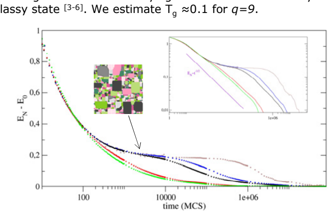
Energy per spin vs. time after a quench from T=∞, for a N=300x300 lattice, at different temperatures ranking from T=0,5 (blue) to T=0,721 (dark green).

For quenchs near T_c the system relaxes to a metastable state from which it escapes mostly through a nucleation process.



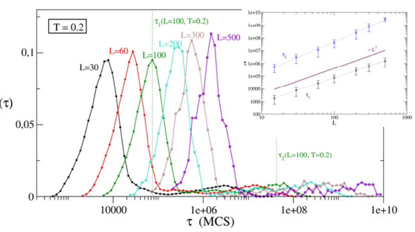
Far enough from T_c we have a typical coarsening behaviour, in the sense that the typical domain length l grows as $l(t)\sim t^{1/2}$, standing that $E_N(t)\sim t^{-1/2}$ and $E_N(t)\sim l(t)^{-1}$ [11]

Below at certain temperature T_g the system develops a pseudo-plateau at low energies. This slow decaying state has been recently associated to a glassy state [3-6]. We estimate $T_g \approx 0.1$ for $q=9$.

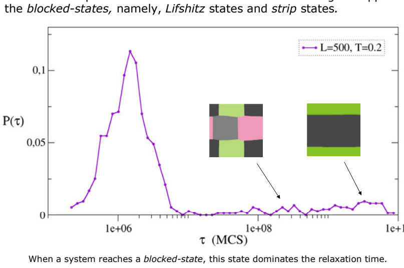


Internal energy per spin vs. time for a N=200x200 lattice at T=0,3(green); 0,2; 0,1; 0,09; 0,07 (brown). The inset shows the log-log scale, and the snapshot is a typical configuration of the system during the namely glassy state.

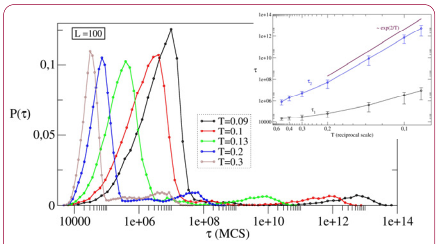
Relaxation time



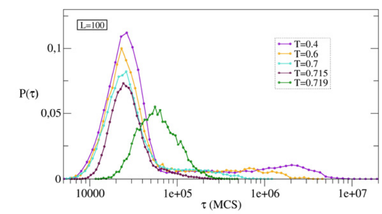
We are able to attribute the first big peak to realizations that follow a *typical coarsening*. If we have $l(t)\sim t^{-1/2}$ and we expect $l(t\approx\langle\tau\rangle)\sim L$, then the mean value $\langle\tau\rangle$ must grow like $\langle\tau\rangle\sim L^2$. The others characteristic peaks are due to those realizations that get trapped in the *blocked-states*, namely, *Lifshitz* states and *strip* states.



When a system reaches a *blocked-state*, this state dominates the relaxation time.

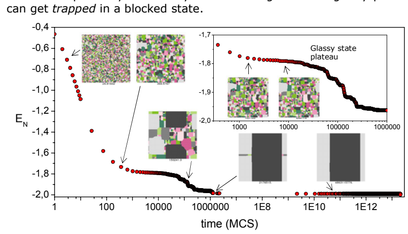


As T decreases an Arrenius-law is satisfied for the mean escape time from a *strip* blocked-state, $\langle\tau_2(T)\rangle\sim e^{\Delta A.J/kT}$, consistently with [7] for the $q=2$ (Ising) case.

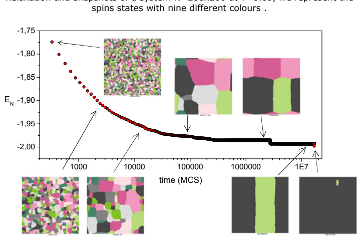


We define T* as the temperature from which we are not able to distinguish different characteristic peaks any more. Blocked-states realizations, if present, unblock quickly at higher temperatures and contribute to the disappearing tail of the distribution.

A system could avoid the blocked-states or get trapped in one or both of them sequentially. Even a system releasing from the glassy plateau can get *trapped* in a blocked state.

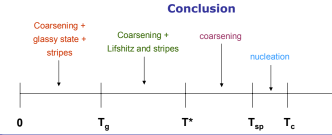


Relaxation and snapshots of a system N=200x200 at T=0.09, we represent the spins states with nine different colours .



Idem, for L=300 and T=0.3

Conclusion



for q=9
T_g ~ 0.1
T* ~ 0.6
T_{sp} ~ 0.715

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