Phase ordering and symmetries of the Potts model

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We have studied the ordering of the q-colours Potts model in two dimensions on a square lattice. On the basis of our observations we propose that if q is large enough the system is not able to break global and local null magnetisation symmetries at zero temperature: when $q < 4$ the system forms domains with a size proportional to the system size while for $q > 4$ it relaxes towards a non-equilibrium phase with energy larger than the ground state energy, in agreement with the previous findings of De Oliveira et al. [11, 12].

Keywords: Phase ordering dynamics; lattice models; non-equilibrium statistical mechanics

1. INTRODUCTION

Phase ordering [1, 2] is one of the important topics in non-equilibrium statistical mechanics. For systems with two coexisting phases the situation is generally well understood from the analytic and numeric points of view [2, 3, 4]. For the Potts model [5] with a $q > 2$-degenerated ground state, the situation is not so clear in general. Also in this case, an Allen-Cahn power-law regime [6] and dynamical scaling relations for the structure factor and for the distribution of domain sizes [7, 8, 9] have been predicted [2] and found numerically [10]. On the other hand, a singular behaviour of the Potts model has been recently observed by De Oliveira et. al. [11, 12] when the degeneracy (q) is large enough: in the thermodynamic limit the model was shown to relax towards a 'glassy', disordered, phase with a non negligible density of defects when it is quenched at zero temperature.

This paper is devoted to discuss some ideas for understanding this glassy phase. In the next section we recall the phase and report new results on the ordering of the Potts model after a quench at low but finite temperature. The system equilibrates locally nucleating domains that eventually become of the size of system. In section 3 we study the $T = 0$ case, and we interpret the impossibility to equilibrate in the thermodynamic limit as an impossibility of breaking the local zero magnetisation. Section 4 is to conclude and summarise the main results.

2. DYNAMICS WITH THERMAL FLUCTUATIONS

De Oliveira et. al. [11, 12] have recently observed an interesting slow relaxation in the dynamics of the Potts model after a quench from a disordered state to zero temperature, and the impossibility for the system to achieve the ground state in the $L \to \infty$ limit, being L the linear size of the system. Let us briefly describe this effect. Given a lattice $\mathbf{L}$, in which each site $i \in \mathbf{L}$ can take q equivalent values, or *colours*, the Potts model [5] is defined by the Hamiltonian:

$$H = \frac{1}{2} \sum_{\{i,j\}} (1 - \delta_{c_i,c_j}) \tag{1}$$

where $\{i, j\}$ means $i \in \mathbf{L}$, j is a neighbour of i, and where $c_i \in \{1 \cdots q\}$ is the colour of site i. When quenching at zero temperature a two-dimensional system on a square lattice using Glauber single spin-flip dynamics, systems with $q > 4$ obey the Allen-Cahn law [2] $e(t) \propto t^{-1/2}$ (e being the energy per site) up to a time $\bar{t}$, increasing with L, when they get trapped in a blocked configuration, invariant with respect to the single spin-flip dynamics at zero temperature [13, 14, 15][23]. Inverting the usual order of the $t \to \infty$ and $L \to \infty$ limits, i.e., assuming that the thermodynamic limit is taken before the infinite-time limit, and extrapolating to $t \to \infty$ the $e(t)$ data with the Allen-Cahn power-law $e(t) \propto t^{-1/2}$ [11], one finds a positive energy $e^* \equiv e(t \to \infty) > 0$ for $q > 4$ and, in particular the data for e^* is very well fitted by the expression $e^* = bL^{-1/2} + b'(q-4)^{1/2}$, b, b' being real constants. This would imply that an infinite-size system with $q > 4$ relaxes after an infinite time towards a phase with stationary observables and positive

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energy, different from the ground state with zero energy, and this is the reason for which this out-of-equilibrium 'phase' is called 'glassy phase' in [12]. A noticeable point is that the onset of this glass-like phase occurs in the two-dimensional Potts model for $q > 4$, and this q-range coincides with the one in which the system presents a first-order phase transition [5]. A justification of this fact is in progress [16]. We now give a general characterisation of the equilibration of the system at finite temperature, and an interpretation of the non-equilibrium phase in terms of the symmetries of the problem in Section 3.

We have studied the dynamics after a quench at finite temperature, $T = 0.1$, of the 7 colours Potts model with periodic boundary conditions, being $T_c = \ln^{-1}(1 + q^{1/2}) = 0.7730...$ the critical temperature of the model [5]. In Fig. 1 we present the energy per site (on top) and the magnetisation (centre) with respect to $t^{-1/2}$ of a 2-d square lattice system with nearest-neighbours interaction and periodic boundary conditions. The magnetisation, m, is

$$m = \frac{q}{q-1}\Big(\sum_c^q x_c^2 - 1/q\Big) \tag{2}$$

where x_c is the fraction of colour c, $x_c = N_c/N$, N_c being the number of sites in the system with colour c and $N = L^2$ is the total number of sites. The magnetisation is zero when $x_c = 1/q\ \forall c$, and one when all spins have the same colour. Initially the system is in an uncorrelated configuration at infinite temperature, with $e = 2(q-1)/q$ and $m = 0$. For $t < \tau$, systems with $q > 4$ coarsen with equal proportion of all colours and with the expected power-law dependence of the energy on time [6] while, for $t > \tau$, finite-size systems equilibrate, breaking the $m = 0$ symmetry and approaching gradually the ground state with $m = 1$, $e = 0$. The above description of the problem suggests that, for $q > 4$ and for times larger than τ, coalescence effects, not considered in the derivation of the Allen-Cahn law, become relevant in the dynamics, and allow the mean domain size, ℓ [2], to grow up to the system size, L. The numerical results reported in Fig. 1 suggest that, for $T > 0$, τ is not divergent in L, but constant above a certain L, i.e., that the "nucleation" needed to equilibrate the system is a local process no longer dependent on L. In fact, the $L = 10^3$ and $L = 500$ curves of Fig. 1 coincide within $\sigma_e^2(t, L)$, the variance of the distribution of energy values corresponding to different realisations of the quench (shown in error bars).

We observe from Fig. 1 that the $m = 0$ symmetry is broken later in larger systems. As in [17] for the continuous Ising model, the magnetisation is supposed to be zero for all times in the absence of finite-size effects, and in fact we find [16] a similar scaling relation $m(t, L) = m(t/L^2, 1)$ for $q = 2, 3$, and even a slower dependence of $m(t, L)$ on L for $q > 4$. One could ask why τ seems to approach a limit value with $L \to \infty$, while the magnetisation at fixed times tends to zero in this limit. To answer this question we propose the following argument: systems with $q > 4$ equilibrate leaving at $t = \tau$ the power-law dependence of the energy on time and forming domains that will eventually become system-sized, and τ seems to be a characteristictime of the model. It is this local nucleation the origin of the ordering, rather than the changes on the global colour fraction, which is a finite-size effect [16]. In order to supply a quantitative support to this argument we define an order parameter, γ, accounting for the spatial ordering, which seems to characterise the dynamical ordering more than the global magnetisation, m [18]. Let us define γ as a distance from the $\mu(\mathbf{r}) = 0$, $\forall \mathbf{r}$, situation, where $\mu(\mathbf{r})$ is the magnetisation of a cell centred in $\mathbf{r}$ and of size λ, independent of L, in such a way that $\lambda/L \to 0$ in the thermodynamic limit. In particular,

$$\gamma \equiv \frac{1}{V}\int d\mathbf{r}\ \mu(\mathbf{r}) = \frac{q}{q-1}\frac{1}{V}\int d\mathbf{r}\ \Big(\sum_c^q \phi(\mathbf{r})_c{}^2 - 1/q\Big) \to \frac{1}{L^2}\sum_{i\in\mathbf{L}}^{L} \mu|_{\text{cell } i}, \tag{3}$$

where V is the volume of the general system and $\phi_c(\mathbf{r}) \in [0:1]$ is the proportion of colour c in the cell centered in $\mathbf{r}$. The expression at the right of the arrow in (3) is the definition of γ in the lattice $\mathbf{L}$ and cell i is a cell centred in the position of site i [24]. For $L \to \infty$, γ so defined is zero in the completely uncorrelated configuration, and one in the ordered configuration, when all the sites have the same colour and $m = 1$. Since $\mu \geq 0$, γ is a distance, functional of $\mu(\mathbf{r})$, and can be used as an alternative order parameter accounting for the spatial ordering of the system. We see in Fig. 1 (bottom) that also γ presents a power-law dependence on time. As expected by the argument exposed above, γ seems not to depend on L for large L: curves for $L = 500$ and 10^3 coincide within their standard deviation limits. Moreover, γ seems to leave the power-law regime and converge to 1 at τ.

3. $T = 0$ DYNAMICS AND SYMMETRIES OF THE GLASSY PHASE

At zero temperature, the situation is different: the above defined time, τ, needed to leave the Allen-Cahn law is divergent with L, as described in [11], and an infinite-size system is always supposed to follow the Allen-Cahn power-law. In larger and larger systems, it is less and less likely to find a blocked configuration or a path in phase space to

the ground state. A measure of this fact can be seen in the value of the energy variance, $\sigma_e^2(t, L)$, which decreases with L (see inset of Fig. 3). This means that in a large system it is less likely to find a deviation from the power-law regime, in which blocked dynamics [13] or breaking of the $m = 0$ symmetry [17] are not present. This explains at a qualitative level the fact that in large systems the magnetisation is broken later (and hence the system equilibrates later), but it does not address the fact that the energy of an infinite size system with $q > 4$ converges to a positive value for $t \to \infty$. In other words, it does not explain why the term e^* of the generalised Allen-Cahn law $e = at^{-1/2} + e^*$ is different from zero for $q > 4$. One could ask why systems with $q > 4$ cannot converge to a zero energy phase in the limit $L \to \infty$, even respecting the $m = 0$ symmetry, as the $q = 2$, 3 cases do. We discuss this point in the following.

Numerical simulations show that in the latest stage of the coarsening at zero temperature, systems with $q = 2$, 3 and with large enough L (to respect the $m = 0$ symmetry) present final configurations formed by domains of the size of system (Fig. 2, left) and $\ell(t)$, the mean domain size, is proportional to L when $t \to \infty$. The energy, or the perimeter of the interface, is proportional to L, and thus, the energy per site is zero in the thermodynamic limit. In fact we have $e^*(q) = 0$ for $q = 2$, 3, as said before. On the other hand, for $q > 4$, we observe that the system presents not only $m = 0$, but also a local symmetry that is a local equal fraction of all colours. We define this local symmetry by introducing a certain scale, λ, with $L > \lambda > \ell$, such that the magnetisation is also zero in every cell of the system of size greater than λ and *being* λ *such that* $\lambda/L \to 0$ *for* $L \to \infty$. We propose, and we argue below, that the zero temperature dynamics cannot form domains of the size of the system for $q > 4$, hence the perimeter of the interface (as well as the final number of domains) grows with L^2 and the energy per site of the glassy phase is not zero in the thermodynamic limit, while, in this limit, systems with $q = 2,\ 3$ do not break the $m = 0$ symmetry when forming domains of the size of the system but they can break the local $m = 0$ symmetry. A numerical confirmation of this argument is that γ converges to $\gamma^* = 1$ in the $L, t \to \infty$ limits for $q = 2,\ 3$, but $\gamma* < 1$ for $q = 7$: the fraction of the volume V for which $\mu \neq 1$ is not negligible in the thermodynamic limit. In Fig. 3 we report the energy, magnetisation and order parameter of local ordering as a function of $t^{-1/2}$ for the $T = 0$ dynamics in the $q = 7$, 3 and 2 cases. It seems that γ presents the same power-law dependence on time as the energy in the $q = 7$ case. Inverting the order of the limits and extrapolating to $t \to \infty$ with a linear fit, as done for the energy in [11], we have $\gamma^* = 0.807 \pm 0.005$, while for $q = 2, 3$, γ converges to 1.

This local zero magnetisation for $q > 4$ (see Fig 2, right) characterises the glassy phase also in the sense that it predicts a $q^{1/2}$ dependence of e^*, which coincides in the $q \to \infty$ limit with the result $e^* \sim (q-4)^{1/2}$ of [11]. Let us show this fact in the approximation of domains of identical size ℓ [19]. In order to satisfy the local-$m = 0$ condition there must be nq domains inside each cell of size λ, n being an integer. In d dimensions it is $e \sim n_D\ \ell^{d-1}/L^d = \ell^{-1}$, where $n_D = L^d \ell^{-d}$ is the number of domains, and setting $\lambda^d/\ell^d = nq$ we have $e \sim \lambda^{-1} q^{1/d}$. When q approaches 4, coalescence effects not considered in this argument become important, to which we attribute the slower dependence on q of the energy, $e^* \sim (q-4)^{1/2}$.

As we have seen there are evidences that, in absence of thermal fluctuations, the Metropolis dynamics cannot break the local symmetry of colours when $q > 4$. This fact and the $q > 4$ limit can be explained (not yet in a rigorous fashion) as a consequence of an assumption on the glassy phase symmetries. To introduce it let us define the q 'coarse-grained' fields $\phi_c(\mathbf{r}) \in [0, 1]$, in analogy with [9], as the fraction of colour c in a cell centred in $\mathbf{r}$ and of size λ. Clearly $\sum_c^q \phi_c = 1$ and the fields ϕ_c describe the configuration in a λ-dependent way. Given the fact that the Hamiltonian is invariant with respect to S_q, the group of permutations of the q colours, we assume that the $m = 0$ symmetric configuration corresponding to $L \to \infty$, $t \to \infty$ is maximally ordered in such a way that any permutation of the colours, $p \in S_q$, is equivalent to a p-dependent global spatial transformation, U_p. i.e.:

$$\phi_{p(c)}(\mathbf{r}) = \phi_c(U_p \mathbf{r}) \qquad \forall p \in S_q \tag{4}$$

If we assume the operator U to be linear we have that $U : S_q \to \mathscr{L}(\mathbb{R}^2)$ is a representation of S_q in the vector space of linear operators in the plane, $\mathscr{L}(\mathbb{R}^2)$. Since there is no representation of S_q in $\mathscr{L}(\mathbb{R}^2)$ for $q > 4$ different from the trivial representation ($U_p = \mathbb{I}$, the identity operator on $\mathbb{R}^2$, $\forall p$), from the above assumption it follows the local-zero magnetisation of the glassy phase for $q > 4$: setting $U_p = \mathbb{I}$ in (4) we obtain $\phi_{c'}(\mathbf{r}) = \phi_c(\mathbf{r})$, that with the normalisation condition gives $\phi_c(\mathbf{r}) = 1/q\ \forall \mathbf{r}, c$, i.e., the local $m = 0$ symmetry in the cell of size λ. The assumption (4) can also 'justify' the spatial symmetries of configurations with $q \leq 4$ in the $m = 0$ regime: for $q = 2$ the group S_2 admits a nontrivial representation in the plane, $\{\mathbb{I}, \alpha\}$, where $\mathbb{I}$ is the identity and α is the rotation of π radians in the polar angle and, in fact, configurations with $q = 2$ in the glassy phase seem to present this symmetry (see Fig. 2, left), and a similar $2\pi/3$ rotational symmetry seem to exist for $q = 3$ configurations, even if it is often hindered by the two-preferred directions of the square lattice interaction [13] and by the formation of structures locally stable under the $T = 0$ dynamics [1, 20]. Moreover, in a general d-dimensional system, there exist no nontrivial representations of S_q in $\mathbb{R}^d$ for $q \geq d + 2$ [22]. This proposition seems to be true for all $q > 4$, and we are working on the general proof. If verified, this consequence of the assumption (4) would coincide with the result by Lifshitz [1], who argued that a

d-dimensional system quenched below its critical point does not necessarily equilibrate into an ordered state, in the presence of a ground state that is degenerated more than $d+1$ times.

4. CONCLUSIONS AND FURTHER RESEARCH

We have studied the ordering dynamics of the 2-d Potts model in a square lattice with $q = 2, 3$ and 7 by use of single-spin flip dynamic Monte-Carlo simulations. At positive temperature, $T = 0.1$, and for $q = 7$ the system relaxes leaving the Allen-Cahn power law at a given time, which is independent on L for large L. At zero temperature, in the $L \to \infty$ limit, systems with $q > 4$ are not able to nucleate breaking the local symmetry, and hence they converge to a phase with nonzero energy. We give a quantitative support for this argument in the $q = 7$ case with the help of an order parameter of local ordering that we define. The $q > 4$ limit is presented as a consequence of a hypothesis on the symmetries of the glassy phase. For both temperatures the magnetisation at equal times decreases with increasing sizes and it is argued to be zero in the thermodynamic limit at any time [17]. A generalisation of this study for different q values and for larger L is being performed [16] together with an investigation of the relation between the ordering properties and the phase space structure.

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[24] In the numerical construction of γ, we have taken the nearest 24 neighbours of each site for the definition of the mentioned cell.

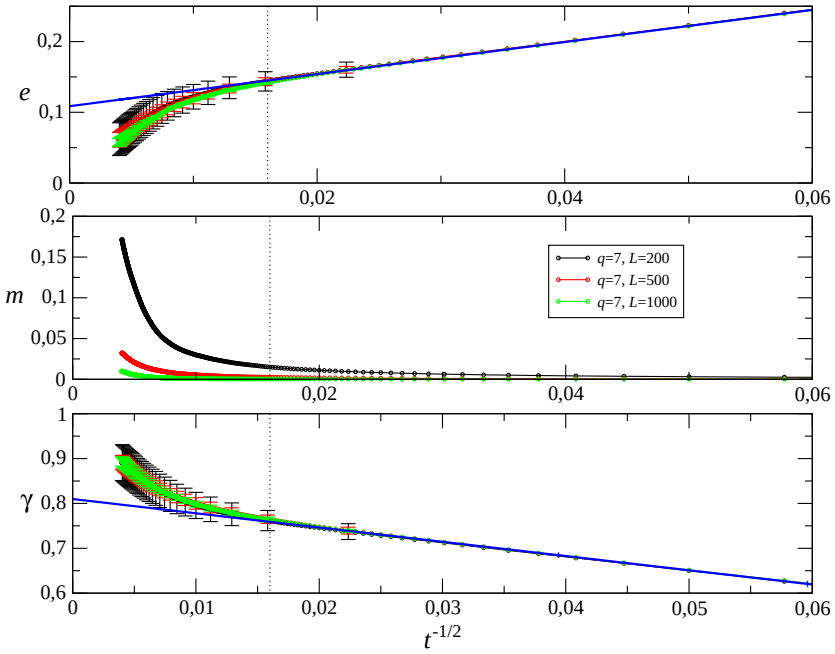
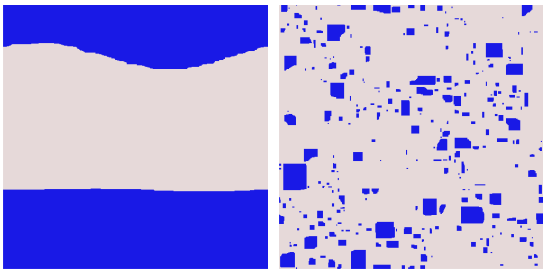


FIG. 1: Energy per site (e), magnetisation (m) and order parameter of local ordering (γ) with respect to $t^{-1/2}$ for the Potts model with $q = 7$ after a quench to temperature $T = 0.1$. Results are averaged over 200, 60 and 30 realisations (for $L = 200$, 500 and 10^3, respectively). Time is in MCS units. Error bars in the y-axes are the variances, σ^2, of e and γ, corresponding to the average over different realisations of the quench (shown every 2000 MCS only). In larger systems the $m = 0$ symmetry is broken later [17]. σ^2 decreases with the size of the system at equal times. The blue line is a fit to the $L = 10^3$ system energy in the range $t^{-1/2} \in [0.02, 0.1]$, and the vertical dotted line is an estimation of the nucleation point, corresponding to the time at which e differs from the fit more than $\sigma_e^2/2$. At that time, τ, the system nucleates leaving the Allen-Cahn power law, and γ increases towards 1.



$q = 2$ $\gamma = 0.992$ $\quad$ $q = 7$ $\gamma = 0.775 < \gamma^*$

FIG. 2: Example of two configurations reached by the 2 and 7-colours Potts in a $L = 500$ lattice, after 6.25 10^4 MCS of a single realisation of a quench at zero temperature. The magnetisation is $m = 1.9\ 10^{-4}$ and $9.6\ 10^{-4}$, respectively. Spins with a given colour are shown in blue, while spins with the remaining $q - 1$ colours are shown in white. In the latest stage of the coarsening the interfaces between domains of the $q = 2$ case become straight lines.

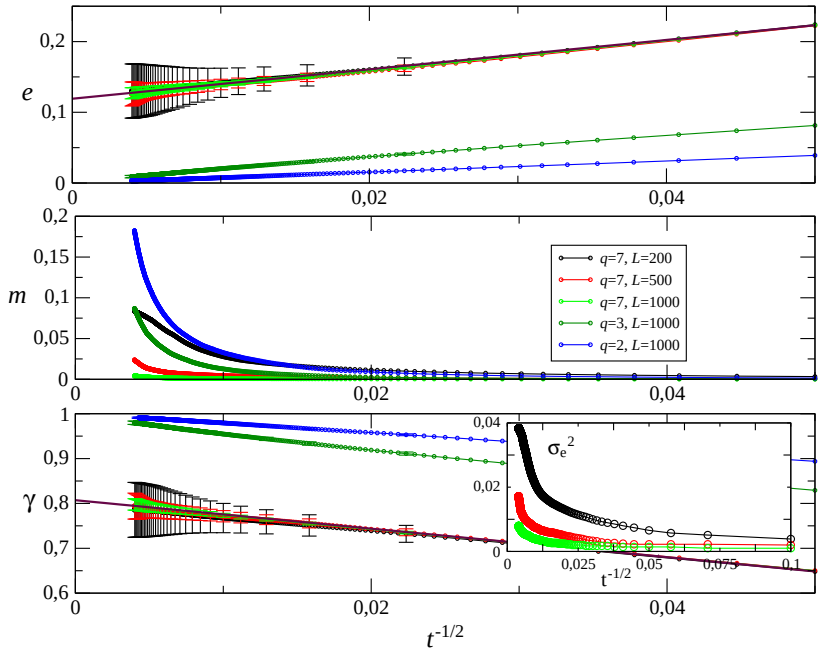


FIG. 3: Energy per site (e), magnetisation (m) and order parameter of local ordering (γ) with respect to $t^{-1/2}$ for the Potts model after a quench at zero temperature. The $q = 7$, 3 and 2 cases are presented, and three different sizes for the $q = 7$ case. Magnitudes are an average over 240, 60 and 40 realisations of the quench in systems with $L = 200$, 500 and 10^3, respectively. For the cases $q = 2$ and 3 the energy converges to zero following the Allen-Cahn law, while in the $q = 7$ case it converges to $e^* = 0.1192$ ([11]). The global magnetisation decreases with q at equal times and sizes, for all sizes and times studied. It also decreases with L for all times [17], and it is supposed to be zero in the thermodynamic limit. Even with this constraint, systems with $q < 4$ can form system-sized domains with zero energy, and in fact they order spatially, and $\gamma(t \to \infty) \to 1$, while the zero-temperature dynamics cannot break the local zero magnetisation symmetry to form domains of the size of the system when $q > 4$, as illustrated by the fact that $\gamma(t \to \infty) \to \gamma^* < 1$ for $q = 7$, and this is the reason for which $e^* > 0$. The extrapolated line is a fit to the $L = 10^3$ data for $0.005 < t^{-1/2} < 0.06$ MCS$^{-1/2}$. The fit coincides with the data within its variance limits. The equation of the fit is $\gamma_{\rm fit} = \gamma^* + at^{-1/2}$ with $\gamma^* = 0.8072$ and $a = -3.1756$. On inset we present the variance σ_e^2 of the energy, which is a decreasing quantity with L, for all times and for the three sizes studied.