

Dynamic metastability in the two-dimensional Potts model

Miguel Ibáñez de Berganza^{§‡*}, Vittorio Loreto[§] and Alberto Petri[‡]

[§]*Dipartimento di Fisica, Università di Roma “La Sapienza”. Piazzale A. Moro 2, 00185 Roma, Italy.*

[‡]*CNR, Istituto dei Sistemi Complessi, sede di Roma 2-Tor Vegata. Via del Fosso del Cavaliere 100, 00133 Roma, Italy.*

We have studied the dynamics just below the temperature-driven critical point of the 2D q -color Potts model in the square lattice, for $q = 8, 12, 24$. For finite-size systems, a metastable quasi-steady regime *à la* Binder is observed, which we characterize by means of the nucleation and relaxation times of the metastable phase. This phase is no longer observed below a given temperature, T_{sp} , at which the relaxation time of the fluid becomes of the order of the times involved on the nucleation processes. However, this temperature, which decreases for increasing q , converges to the critical temperature of the model for increasing sizes and fixed q , and no metastability is supposed to exist in the thermodynamic limit. These results agree with the droplet expansion performed for the 2D Potts model by Meunier and Morel [16].

Keywords: non-equilibrium statistical mechanics; dynamic metastability; Potts model

I. INTRODUCTION

When a liquid is cooled below its melting temperature, crystallisation can often be avoided by a fast enough cooling, and the liquid enters a phase, called supercooled [1, 2, 3]. The supercooled phase is *metastable*, it has a finite lifetime and it is unstable with respect to large fluctuations although those characteristics are not a practical limitation: metastable states are ubiquitous in nature and in technology (see references in [2]), and not distinct from stable states under many practical respects. Metastability, as a general concept, is present in many fields of physics, from superconductivity to high-energy physics (see references in [4]). In particular, the understanding of metastability is crucial in the context of the study of the glass-transition [1, 2, 3, 5]: the structural glass transition occurs, during the cooling process, at a certain temperature below which the liquid falls out-of-equilibrium and forms the structural glass, unstable with respect to the metastable phase. However, and despite of its ubiquity and intrinsic theoretical interest, metastability is still not well understood, and a lot of theoretical effort has been given on the problem in the last decades [4, 6].

From a purely thermodynamic point of view, metastable states satisfy the Callen minimum energy principle, but only with respect to small enough fluctuations. In the thermodynamic space (T, h) of field variables, where T is the temperature and h is the pressure, in the case of a fluid, or the magnetic field, in the case of a magnet, the metastable phase is described by a free energy $f^m(T, h)$ in a region of (T, h) space in which it coexists with the stable phase, described by $f(T, h)$, and it is: $f < f^m$. Metastable states satisfy the local stability condition, $(\partial_{hh} f^m)_T \leq 0$, which is a necessary, but not sufficient condition for stable equilibrium: it only guarantees the stability with respect to infinitesimal fluctua-

tions. Metastable states are not stable with respect to a large enough fluctuation: the system would prefer indeed the equilibrium phase at (T, h) described by $f(T, h)$ since $f(T, h) < f^m(T, h)$.

Statistical mechanics of systems in mean field approximation, as the Landau theory of magnetism or the van der Waals equation of state for the gas-liquid condensation, accounts for metastable phases, which, in this context, exhibit the thermodynamic properties described above. In mean field, the only allowed form of fluctuation is a spatially uniform change of the order parameter, m , and the free energy cost of such a change is extensive in the volume. For this reason, the free energy barriers separating the relative minima of the free energy functional in (T, m) space from the absolute minima, the stable phase, are infinite in the thermodynamic limit, and, hence, the corresponding metastable states would have an infinite lifetime.

When fluctuations are taken into account, however, statistical mechanics of short-range interaction systems cannot account properly for metastability, since, when the thermodynamic limit is taken, the partition function in ensemble theory is dominated by the global minimum of the free energy functional in phase space. Metastable states being not ergodic, they are not well-described by the partition function; for them, temporal averages are not equivalent to the ensemble average. Beyond mean field, there always exist a finite probability of surmounting the free energy density barriers in phase space by a local nucleation process and, hence, it is not possible to state whether a given distribution is metastable without making reference to a timescale, related in some way to the mentioned probability of nucleation [7].

An alternative is the dynamic description of metastability [6, 7, 8], which is characterized by a two-step relaxation during the dynamic evolution of the system in the coexistence region. The two-step relaxation is associated with two times (τ_R and τ_N), such that the order parameter and other observables are quasi-stationary in time in the interval $\tau_R < t < \tau_N$). For systems with discrete phase space, nucleation times can be computed by the

*miguel@pil.phys.uniroma1.it (corresponding author)

numerical solution of a master equation describing their temporal evolution, as pioneered by Binder for the Ising model [4, 8].

Although this dynamic definition of metastability is apparently different from the thermodynamic picture mentioned above, there exist connections between the partition function-based methods and the dynamic considerations [4, 6]. The most relevant is probably the result by Langer [9], who shows that, for a wide class of models, whose dynamics can be described by a Fokker-Plank equation, the nucleation rate, $\Gamma \propto \tau_N^{-1}$, (the number of nucleation events per unit time and volume) can be written under certain limits as:

$$\Gamma = \frac{\beta\kappa}{\pi} |\text{Im } \tilde{f}| \quad (1)$$

where $\beta = 1/kT$ is the inverse temperature, the prefactor κ contains all dependence on the specific dynamics, and $\text{Im } \tilde{f}$ is the imaginary part of the (divergent) analytical continuation of the equilibrium free energy density in the region of (T, h) corresponding to the ordered state. This puts into relation and generalizes several other previous results, as the Arrhenius-like relation $\ln \Gamma(T, h) = \ln c(T) - \beta F(T, h)$ between the nucleation rate and the free energy cost, F , of the formation of a ‘critical droplet’, in the context of classical nucleation theory [4, 10], giving also the expression for c from first-principles.

There are also other connections between ‘static’ and dynamic approaches to metastability, as the result by Penrose for the droplet model of condensation [11] (see also [6, 12]), a gas of non-interacting droplets of all possible sizes. If the partition function is restricted to consider only undercritical clusters, nucleation is avoided, and analytic continuations of stable isotherms in the metastable region can be computed. The resulting free energy, moreover, coincides with $\text{Re } \tilde{f}$, and also the Langer relation between $\text{Im } \tilde{f}$ and Γ holds when the Becker-Döring dynamic is considered for the droplets [10].

Even if the result (1) by Langer has been proved for several models (see references in [4]), no general proof exists, and its validity is unclear [14]. In particular, the identity (1) has been proved [12] for the field-driven transition of the Ising model below the critical temperature and in the limit of small field, computing \tilde{f} from a droplet expansion.

For this model it has been shown the equivalence between both types of calculations of Γ , using the field-theoretical calculus of \tilde{f} , and the solution of the Master equation with the Monte-Carlo method [8]. This agreement has been extensively further studied for the Ising model [15]. Lattice models are particularly suitable for this comparison since, on the one hand, it is possible to compute numerically nucleation rates, and, on the other hand, their critical properties and surface tension are often known exactly, which makes possible an analytical droplet expansion calculus. Moreover, as mentioned in

[8], the concept of droplet is for them unambiguously defined.

A similar droplet expansion computation of the free energy has been done in 2000 by Meunier and Morel [16] for the study of the first-order transition of one of the better known lattice models in equilibrium statistical mechanics: the q -color Potts model (q -PM) with $q > 4$ [17]. For finite-size systems, a free energy barrier is found, associated with a metastable state, in a given temperature range, which is shown, however, to shrink to zero in the thermodynamic limit. To our knowledge, the present work is the first attempt to contrast the results of Meunier and Morel with a dynamic computation, as they suggest to do.

Nevertheless, the dynamics associated with the q -PM transition has already been studied [18, 19, 20, 21, 22, 23, 24], and it is itself a topic of relevance. In [18] metastability in the field-driven transition of the 2d q -PM is studied. Numerical results suggest the existence of a dynamic metastable phase associated with the temperature-driven transition for $q = 5, d = 2$ and $q = 3, d = 3$ [19, 20], even if such a metastable phase is not analysed quantitatively. For this transition hysteresis cycles are studied numerically, in [22, 23], and it is concluded that relaxation through the equilibrium state occurs via nucleation. In this work we present some results on the dynamic metastability of the q -PM in the lattice, emphasizing its dependence on the lattice size, up to a linear size $L = 375$. In the next section we introduce the model and our notation, the previous results of the droplet expansion [16] and of the mean field approximation for the model. In section III we present and interpret the results from the dynamics, together with the finite-size analysis, and compare them with those introduced in section II. Section IV is to conclude and summarize.

II. MEAN FIELD AND DROPLET EXPANSION

The Potts model [17] is defined in a lattice \mathbf{L} in which every site, $i \in \mathbf{L}$, can take q equivalent values, $c_i \in \{1 \dots q\}$, usually called *colors*. The Hamiltonian is:

$$H = \frac{1}{2} \sum_{\substack{i \in \mathbf{L} \\ j \in \mathbf{N}(i)}} (1 - \delta_{c_i, c_j}) \quad (2)$$

where $\mathbf{N}(i) \subset \mathbf{L}$ is the set of neighbours of the site i . The model has been proved [17, 25] to exhibit a first-order phase transition for $q > 4$ in two dimensions, and a continuous phase transition for $q \leq 4$. In the square lattice both transitions occur at a critical inverse temperature $\beta_c(q) = \ln(1 + q^{1/2})$. The $q = 8, 12, 24$ -color Potts models we study are, thus, 2d-lattice models, with short-range two-body interactions and which presents a first-order temperature-driven transition at $\beta_c(q)$.

In the absence of external fields, the q -PM has only two thermodynamic variables, (T, N) , N being the number of sites, and the reduced equation of state is $df(T) = -s(T) dT$. The mean field approximation [17] predicts a first-order transition for $q > 2$ at a temperature $T_c = \gamma(q-2)/(q-1) \ln(q-1)$, where γ is the connectivity. The equilibrium state for $T > T_c$ is the disordered state with zero magnetization ($m = 0$): it is the absolute minimum of the free energy functional, φ in (T, m) space. For undercritical temperatures, the absolute minimum is no longer the disordered state, but there still exists a local minimum at $m = 0$, which can be associated to an undercooled, metastable disordered state, and which survives in the temperature range $T_c > T > T_s = \gamma/q$ since, in this interval, it is $\partial_m \varphi|_{m=0} = 0$ and $\partial_{mm} \varphi|_{m=0} > 0$.

The droplet expansion performed in [16] predicts, however, a disappearance of the metastable range in the thermodynamic limit. The free energy of the disordered phase is computed from the following series, in which each term is the free energy of clusters of area ℓ ([10, 16]):

$$F(\beta) \propto \sum_{\ell=1}^{\infty} \ell^{-\tau} e^{(\beta-\beta_c)\ell - \omega\ell^\sigma} \quad (3)$$

being ω the interface tension and σ, τ non-geometrical exponents discussed in the work. Replacing the discrete sum by an integral, and making certain assumptions on the form of the interface tension from previous known results, an expression for the free energy of the disordered phase is found and compared with numerical data for the free energy cumulants. From this free energy and for finite-size systems of area A , a probability distribution, $P_{\beta_c, A}(e)$, for the energy at the critical point is also found. It is possible to obtain a former probability distribution, $D_{\beta, A}(e)$, for temperatures lower than the critical point, by a reweighting of P . $\ln D_{\beta, A}(e)$ is proportional to the free energy functional φ_A in (β, e) space. In finite-size systems, a local maximum of $\ln D$ with high energy exists for undercritical temperatures. It corresponds to a metastable state, different from the global maximum, corresponding to the ordered phase at low energy. Metastability is characterized by a barrier separating the local and global maxima of $\ln D$, which ends at its local minima, and by a ‘‘spinodal temperature’’ below which the barrier disappears. Due to the singular behavior of the free energy at β_c , D is strongly size dependent for $\beta > \beta_c$ and e lower than the equilibrium energy at β_c , and this fact leads to a shrinking of the metastable range to zero for large sizes: the spinodal temperature converges to β_c .

In subsection III C we compare the properties of this spinodal temperature with the one we find in our dynamic analysis.

III. DYNAMIC ANALYSIS

A. Method and general features of the dynamics

The dynamic evolution of the model is studied using the single-spin dynamic Monte-Carlo method to solve the time-discretized Master equation for the probability $P(\mathbf{C}, t)$ of the system to be in a given color configuration, $\mathbf{C} = \{c_i\}_i$, at time t :

$$\frac{d}{dt} P(\mathbf{C}, t) = \sum_i^N \sum_c^q \{P(\mathbf{C}_{c_i \rightarrow c}, t) \omega(i, c_i, \mathbf{C}_{c_i \rightarrow c}) - P(\mathbf{C}, t) \omega(i, c, \mathbf{C})\} \quad (4)$$

where $\omega(i, c, \mathbf{C})$ is the rate of changing the color i into color c , and $\mathbf{C}_{c_i \rightarrow c}$ is the configuration \mathbf{C} with the i -th spin flipped to colour c . The expression for the transition rates we use is the Metropolis rule [4, 26], $\omega(i, c, \mathbf{C}) = \min\{1, e^{-\beta \Delta E}\}$, where $\Delta E = H[\mathbf{C}_{c_i \rightarrow c}] - H[\mathbf{C}]$ is the energy change of the flip, and $H[\mathbf{C}]$ is the energy of the configuration \mathbf{C} , eq. (2).

In this work we have studied the dynamics of the model with $q = 8, 12, 24$ in 2d-square lattices of linear size $L = 62, 125, 250, 375$, $N = L^2$ sites, and periodic toroidal boundary conditions. In Fig. 1 we show the energy per site, e vs. time for the dynamics at several values of the inverse temperature β , just above the critical inverse temperature β_c , in a system with $q = 24$, $L = 125$. A completely uncorrelated configuration is used as initial condition. We average the energy over different realizations of the initial condition and of the random sequence used in the Metropolis algorithm, and the result is the energy per site e . In other words, $e(t) = \sum_{\{\mathbf{C}\}} P(\mathbf{C}, t) H[\mathbf{C}] / N$, with P from Eq. (4).

For low enough β , the two-step relaxation, characterizing dynamic metastability [6, 8], is observed. Single realizations of the quench remain in a stationary phase, in which the temporal average of the energy (v. inset of Fig. 1) is constant, up to a certain time. Let us call $\tau_N(q, \beta, L)$ the realization-averaged time taken by the system to nucleate, i.e., to escape from the metastable phase and its corresponding plateau and such that it achieves the equilibrium energy of the ordered state at β for $t \gg \tau_N(q, \beta, L)$.

The inset of Fig. 1 reports the behavior of two realizations, one featuring the nucleation event and one remaining in the metastable phase up to $2 \cdot 10^5$ Monte-Carlo Steps per Site (MCSS) at $\beta = \beta_c + 0.015$. We see that for the three inverse temperatures closest to the critical one, almost no realization nucleates up to 10^5 MCSS (i.e., it seems that $\tau_N(q, \beta, L) > 10^5$ MCSS for $(\beta - \beta_c)/\beta_c < 0.011$ while, the lower the temperature, the shorter is the average nucleation time τ_N taken by the system to leave the metastable phase.

From Fig. 1 and from the analysis of the single realizations, we observe that still at $(\beta - \beta_c)/\beta_c \sim 0.017$

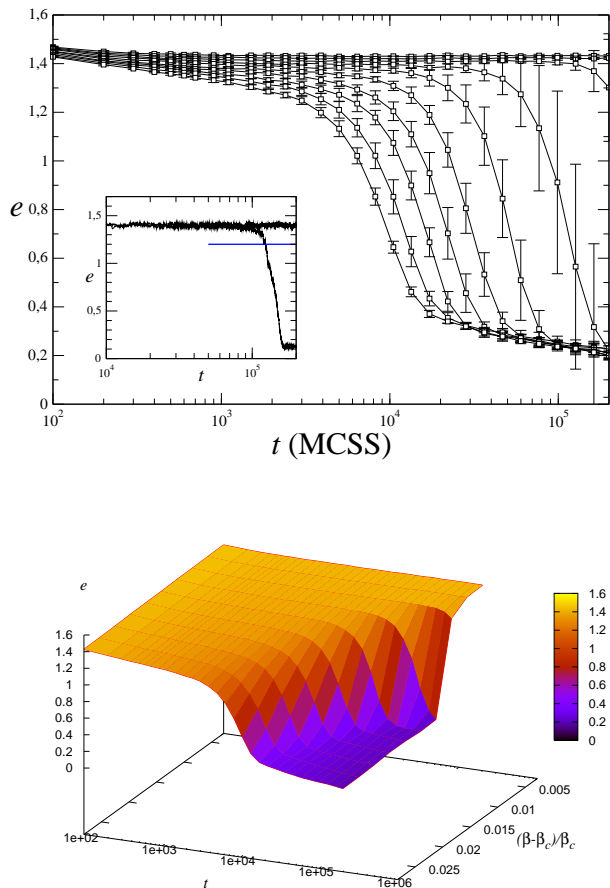


FIG. 1: (color online) Energy per site (e) vs. time (t) of the 24-color Potts model in an $L = 250$ lattice after a quench to different inverse temperatures $\beta_i = \beta_c + 0.005 i$, $i = 1, 2, \dots, 10$. In inset we show two particular realizations of the quench at $\beta = \beta_c + 0.015$, one which nucleates and the other one which does not, up to $2 \cdot 10^5$ MCSS. The horizontal (blue) line is at $e^{thr} = 1.2$ (see text). Error bars are the variance over the set of different realizations.

there are some realizations of the quench which present a very brief stationary phase. For $(\beta - \beta_c)/\beta_c = 0.020 \pm 0.0028$ this regime is no more observed, so we can roughly say that the metastable phase exists in the inverse temperature range $[\beta_c(q), \beta_{sp}(q, L)]$ with $1.017 < \beta_{sp}(q, L)/\beta_c(q) < 1.02$ for $q = 24$, $L = 250$. The so estimated spinodal inverse temperatures are shown as vertical segments in figure 3 for all the q and L studied values, and compared with the ones computed as we will describe in subsection III B.

This picture corresponds to the dynamic metastability limit [1, 27], occurring at a temperature $T_{sp} < T_c$. Let, again, be $\tau_N(T)$, $T < T_c$, the time, averaged over realizations and initial configurations, taken by the system to nucleate when it is prepared in a configuration compatible with the metastable state at T , and when it evolves with the dynamics at T . If $\tau_R(T)$ is the relaxation time of the disordered phase, then we

have that, for the metastable phase to be observed at a temperature $T < T_c$, the nucleation time must be much larger than the time of equilibration of the liquid, $\tau_N(T) > \tau_R(T)$. When lowering the temperature the relaxation time increases while, conversely, it is possible that the metastable phase becomes more and more unstable, and the nucleation time decreases. This behaviour leads to a temperature, the spinodal temperature, T_{sp} for which $\tau_N(T_{sp}) = \tau_R(T_{sp})$, and below which the supercooled phase cannot be conceived due to the fact that crystal nucleation becomes faster than the equilibration of the liquid in the supercooled phase. From a general point of view, this is important as far as, in this circumstance, the existence of a supercooled phase under T_{sp} , and of the corresponding glass, unstable with respect to it [1], are limited by pure dynamical reasons; this dynamic limit to metastability is presented [27] as a possibility of avoiding the Kauzmann paradox, not related to the Adam-Gibbs-Di Marzio picture (see [1, 2]), a possibility already mentioned by Kauzmann himself [5]. To avoid, on the other hand, this kinetic limitation, allowing the existence of the glass at every temperature, we would need $\tau_N(T) > \tau_R(T)$ for every temperature under the critical temperature, and in this way we would have glass, supercooled and crystal phases well defined dynamically at a time t , and characterised, respectively, by the conditions $t < \tau_R$, $\tau_R < t < \tau_N$, $t >> \tau_N$. The condition $\tau_N(T) > \tau_R(T)$ to be satisfied for arbitrary low temperatures, however, would require the nucleation time to have a minimum at a certain temperature, below which it increases with decreasing temperature [1]. Although this is not observed in our under-critical region, where metastability is present, a similar process, or a slowing down of the dynamics for decreasing temperature, is observed in the q -PM model, but at very low temperatures [28, 29], well far the metastable region, when the coarsening with highly localized domain walls dominates the dynamics, and where this temperature-decreasing “nucleation time” would no longer correspond to a nucleation from a metastable phase, that was already suppressed at the much higher temperature T_{sp} .

In our undercritical region, we observe, indeed, for finite size systems, the opposite situation, or the kinetic limit to metastability. This phenomena has been recently observed by Cavagna *et. al.* [27] in a lattice model with short range 5-body interactions and no quenched disorder. In [27], it is also discussed whether a lattice model with no *a priori* disorder can reproduce the characteristic features of structural glasses and reproduce such a kinetic spinodal temperature. In this work we give numeric evidence that an effective spinodal temperature is also present in the finite-size versions of the q -PM (see the finite-size analysis in subsection III C). In analogy with the work of Cavagna *et. al.* [27], we then now perform a study of nucleation and relaxation times, and we will show how, for a system of a given size, L , with $L = 62, 125, 250, 375$, the spinodal inverse temperature, $\beta_{sp}(q, L)$ estimated (as done above for $q = 24$, $L = 125$)

from the analysis of Fig. 1 coincides with the temperature at which the condition $\tau_N \sim \tau_R$ is satisfied.

It may be important to emphasize, however, that the concept of spinodal temperature, below which no realization of the quench is metastable, is not well defined beyond mean field: fluctuations make the transition from metastability to non-equilibrium something depending on the realization, even in the thermodynamic limit. See at this respect the work [30], where the ‘spinodal’ field for the Ising model first-order transition is computed as the field at which half of the computed realizations surmounted a free energy barrier during its path in phase space from the metastable initial condition to the stable state. The crossover from non-equilibrium to metastability, however, is expected to be very sharp, and this assumption allows our definition of spinodal temperature.

B. Nucleation and relaxation times

We now present the computation of the nucleation and relaxation times in the metastable plateau described in the previous section, and computed from the data there presented.

The relaxation time of the liquid, both stable and metastable, can be characterized by means of the temporal single-site correlation function, C , as the characteristic time below which C decreases very fast. The correlation function for the model is:

$$C(t, t_w) = \frac{q}{q-1} \left\langle \frac{1}{N} \sum_i \delta_{c_i(t_w), c_i(t+t_w)} - 1/q \right\rangle \quad (5)$$

where the average $\langle \rangle$ is over different realizations of the quench. In equilibrium, stable or metastable, C is no longer function of t_w (differently from what happens when $T < T_{sp}$, when all realizations break time-translational invariance), and has a characteristic time that seems to diverge (see below) at a temperature lower than the critical temperature. The fit of C with a stretched exponential function, $C(t) = \exp(-(t/\tau)^\gamma)$ is good for all temperatures higher than the critical temperature. However, in the metastable region, $C(t)$ behaves differently from a stretched exponential for small times, and the relaxation time, computed from such a fit, supposes an underestimation of the relaxation time, τ_R . For this reason, we estimate τ_R as the time, averaged over realizations, taken by the temporal correlation function to decrease to a given threshold, C^{thr} . Varying this value from $C^{thr} = 10^{-2}$ to $5 \cdot 10^{-4}$ the obtained relaxation time curves are similar. We set from now on $C^{thr} = 5 \cdot 10^{-3}$.

In Fig. 2 we show τ_R so computed for different inverse temperatures. The results of Fig. 2 indicate that $\tau_R(q, \beta, L)$ is a decreasing function of q , and an increasing

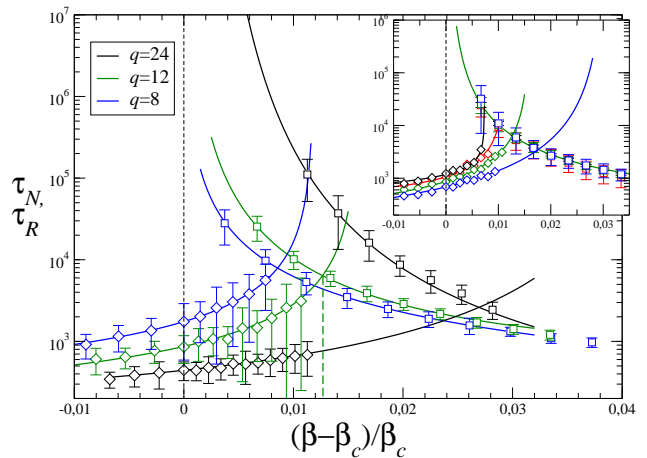


FIG. 2: (color online) Relaxation and nucleation times, τ_R and τ_N (the latter for $\beta > \beta_c$, squares) of the metastable phase for $q = 8, 12, 24$ (decreasing relaxation times) and $L = 125$. Continuous lines are fits with the function $f(\beta) = a \exp(\delta(\pm 1/(T - T_0))^\gamma)$. The vertical black line marks the critical point. From this data, $\beta_{sp}(q, L)$ is estimated as the inverse temperature at which the fits of τ_N and τ_R cross (the vertical green line shows this point for $q = 12$). On inset we show nucleation and relaxation times for $q = 12$ and $L = 62, 125, 250, 375$ (increasing τ_R). For clarity, τ_R error bars are not shown on inset. The data of τ_N do not correspond to the nucleation time for $\beta > \beta_{sp}$, region in which the metastable phase does not exist any longer (see text).

function of L and β , in the studied intervals. Below the critical temperature, it seems to diverge at a low temperature: its T -dependence can be fitted with the function $\exp(\delta/(T_0 - T)^\gamma)$ [1, 27].

Figure 2 also shows the nucleation time. It is estimated as the average time taken by the system to leave the plateau, and decrease in energy until a given threshold, $e^{thr}(q)$. This approximation for the estimation of the nucleation time assumes that the average time taken by the formed critical droplets (at $t = \tau_N$) to grow until the energy has reached the threshold, is negligible with respect to τ_N itself [4]. We have set $e^{thr}(q)$ below the plateau energy, at a distance which is roughly three times the variance of this energy (error bars of Fig. 1). Again, the computed spinodal temperature is not sensible to the choice of $e^{thr}(q)$ if one varies its value in an interval of radius 10^{-2} .

According to this data we can state that $\tau_N(q, \beta, L)$ seems to diverge in the $\beta \rightarrow \beta_c$ limit, with a law of the type $a \exp(\delta/(T_c - T)^\gamma)$, and that, near the critical temperature, it decreases with q and L (see the next subsection for an analysis of these facts from the point of view of the work of Meunier and Morel).

The β -dependence $\exp(\delta/(T_c - T)^\gamma)$ of τ_N can be justified with nucleation theory if one assumes that the bulk free energy density between metastable and stable phases, Δ , is proportional to $\beta - \beta_c$. The free energy cost related to the formation of a d -dimensional droplet of radius R and volume $V(R)$ can be written in nucleation theory as $F(R) = V(R) \frac{d-1}{d} \omega - V(R) \Delta$ and, for a critical droplet,

it is:

$$F_c = \left(\frac{d-1}{\Delta}\right)^{d-1} \left(\frac{\omega}{d}\right)^d. \quad (6)$$

If now one sets: $d = 2$, $\Delta \propto \beta - \beta_c$, and $\tau_N \propto \exp \beta F_c$, it is, for some δ , $\tau_N \propto \exp(\delta/(T_c - T))$.

As explained in section III A, the spinodal temperature can be defined with the condition $\tau_N(T_{sp}) \sim \tau_R(T_{sp})$. In Fig. 2, the dotted vertical line indicates for $q = 12$ the spinodal inverse temperature β_{sp} , at which the fits of the functions $\tau_R(q, \beta, L)$ and $\tau_N(q, \beta, L)$ cross. The results for β_{sp} are presented in Fig. 3 and analyzed in section III C.

It is important to stress that, as already said in sec III A, the data of τ_N do no longer correspond to the nucleation time for inverse temperatures larger than the spinodal inverse temperature, for which the metastable plateau does not exist. In this regime, neither τ_R corresponds to the relaxation time of the metastable phase, and its value may depend on the chosen time in which it is measured, since the temporal correlation function does not satisfy time-translation invariance, i.e., $C(t, t_w)$ may depend on t_w .

C. Finite-size study

From Fig. 3 one can see that β_{sp} decreases with L in the studied interval. The linear fit of Fig. 3 can be taken as a numerical evidence of the fact that the spinodal temperature converges to the critical temperature in the large- L limit. On the other hand, we see that $\beta_{sp} - \beta_c$ increases with q for equal sizes.

These two facts can be justified with the droplet expansion. The convergence of the spinodal temperature to the critical temperature is one of the main results of [16] (see sec. (5.1)). The increasing of the metastable interval for increasing q can be viewed from the form of the probability distribution $D_{\beta,A}(e)$ mentioned in section II (from sec. 4.2 of [16]). For $\beta < \beta_c$, it is (rescaled for all $q > 4$):

$$D_{\beta,A}(\epsilon) = A_r^2 \frac{2}{3} (A_r |\epsilon|)^{-7/3} \exp(- (A_r |\epsilon|)^{2/3}). \quad (7)$$

$\exp A_r \epsilon z$

where $\epsilon = a\xi(q)^{1/2}(e - e_{eq})$, $A_r = a^{-1}\xi(q)^{-2}A$ and $z = \xi(q)^{3/2}(\beta - \beta_c)$ are the rescaled energy, system area and temperature, respectively, $\xi(q)$ is the critical correlation length of the q -PM [25], e_{eq} is the equilibrium critical energy and a is a constant in q and β . Equation 7 is only valid for $e < e_{eq}$. The logarithm of D is proportional to the free energy functional in (T, e) space. The second line of (7) is the β -dependent reweighting, which leads, for large enough $|z|$ to the local minimum of D characterizing

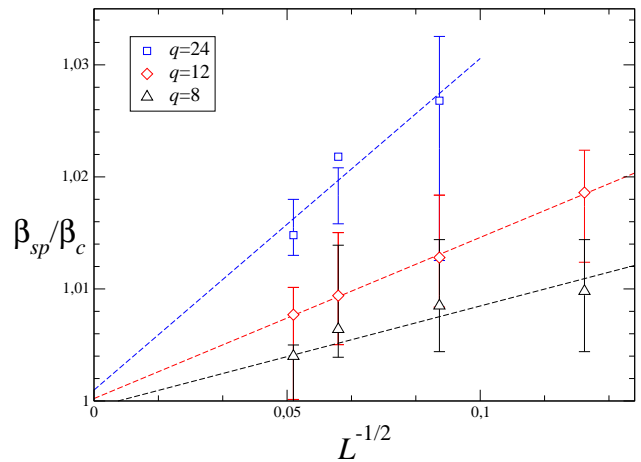


FIG. 3: (color online) Spinodal inverse temperature, β_{sp} , computed as described in caption Fig. 2, for all the studied q 's and sizes. The fit is linear and can be taken as an evidence of the fact that the spinodal temperature converges to β_c in the large L limit. Vertical segments are the estimation of $\beta_{sp}(q, L)$ computed as described in subsection III A: the inverse temperatures above which the plateau is no longer observed. The agreement between the two ways of estimating β_{sp} can be noticed.

metastability, at, say, $e = e_m(z)$. This minimum is at a rescaled energy $\epsilon_m \equiv a\xi(q)^{1/2}(e_m - e_{eq})$ such that the derivative of the logarithm of D in (7) is zero:

$$\frac{7}{3}|\epsilon_m|^{-1} + \frac{2}{3}A_r|\epsilon_m|^{-1/3} = A_r|z| \quad (8)$$

or, in non-rescaled variables:

$$\frac{7}{3}|e - e_{eq}|^{-1} + \frac{2}{3}A^{2/3}\xi(q)^{-1}|e - e_{eq}|^{-1/3} \propto A|\beta - \beta_c|. \quad (9)$$

We see that for increasing q 's the minimum e_m occurs at larger values of $\beta - \beta_c$, since ξ is a decreasing function of q . The spinodal inverse temperature is the β value for which e_m coincides with the inflexion point, e^* , of the functional free energy, $e_m < e^* < e_{eq}$ and above which the local minimum of D is no longer found (see [16]). As far as this inflexion point does not depend on q , also the metastable range $\beta_{sp} - \beta_c$ increases with q .

Assuming the Arrhenius hypothesis mentioned in the introduction, the lifetime of the metastable phase is proportional to the barrier between the metastable maximum and the local minimum of $\ln D$, as said in sec 5.1 of [16]. In the $z \rightarrow^+ 0$ limit, the minimum $\epsilon_m(z)$ in (8) diverges with a law: $A_r|\epsilon_m| = (\frac{2}{3})^3|z|^{-3}$, and $D_{\beta,A}(\epsilon_m(z))$ converges to zero in this limit. Thus, the difference between the $\ln D$ values in the metastable maximum and in the local minima at $\epsilon_m(z)$ diverges for $z \rightarrow 0$, and this justifies the divergence of the nucleation time in the limit $\beta \rightarrow^- \beta_c$ found by us numerically (see Fig. 2).

The minimum of $\ln D_{\beta,A}(e)$ is at the energy e_m at which critical droplets are formed. For temperatures near the critical point, this energy becomes very low, and the time needed for the formation of droplets of such a low energy diverges. On the other hand, for lower temperatures e_m increases and the size of the critical droplets decreases, in such a way that near T_{sp} the time required for the formation of critical droplets is lower than the relaxation time of the fluid, and metastability disappears.

Finally, we see from (9) that, for fixed area and temperature, e_m decreases for increasing q . Since D decreases with q for fixed area and temperature and increases with e for $e_m < e < e_{eq}$, then we have that $D_{\beta,A}(e_m(\beta))$ is a decreasing function of q . Using the Arrhenius hypothesis between free energy barriers and escape times, this justifies the increasing behavior of τ_N with q for equal temperatures and system sizes observed in Fig. 3.

In agreement with [16], these results seem to confirm that metastability in this model is essentially different with respect to the field-driven transition Ising case, in what concerns its dependence on system size (see [31]), and also with respect to the diamond-graphite paradigm. The fast vanishing of the metastable regime presented here can be understood as a call to caution when interpreting hysteresis cycles performed for the q -PM in past or future articles: if the step in β , $\Delta\beta$ of the cooling at a rate $\Delta\beta/\Delta t$ is larger than the corresponding size-dependent metastable interval $\beta_{sp} - \beta$, then none of the points of the hysteresis diagram would correspond to metastable states, but rather to heterogeneous, non-equilibrium configurations, which have already nucleated.

IV. CONCLUSIONS AND FURTHER RESEARCH

We have studied the metastable dynamics of the two-dimensional q -state Potts model ($q = 8, 12, 24$) for temperatures below the critical point, by means of a Monte-Carlo algorithm with local Metropolis updating rule. We observe, for sufficient high temperature,

the energy plateau and the two time-scale relaxation characterizing dynamic metastability. In systems of finite size, L , this phase is described by the functions $\tau_N(q, \beta, L)$, $\beta_{sp}(q, L)$, which are, respectively, the nucleation time and the limit of the supercooled phase, below which the system is no longer stationary nor time-translational-invariant. Our numerical simulation provides a set of values of the mentioned functions, from which we obtain their properties, that we summarize below. *All of them* are in agreement with the results obtained from the droplet expansion for the 2d-Potts [16].

1. $\tau_N(q, \beta, L) \rightarrow \infty$ for $\beta \rightarrow^+ \beta_c$.
2. $\tau_N(q, \beta, L)$ increases with q .
3. $\beta_{sp}(q, L)$ decreases for increasing L , and seems to converge to $\beta_c(q)$ in the large- L limit.
4. $\beta_{sp}(q, L)$ increases for increasing q .

We propose to perform a systematic quantitative comparison between nucleation times and metastability limits computed dynamically and the ones predicted by the droplet expansion, or by a restricted-partition function analysis. We also propose to improve the measure of τ_N by analyzing nucleation effects locally, i.e., formation of critical droplets.

V. ACKNOWLEDGEMENTS

M. I. would like to acknowledge the very useful discussions on metastability with Andrea Cavagna, Pablo Hurtado and Alessandro Attanasi; the hospitality of the Statistical Physics Group of the University of Granada, where the final part of this work was performed; José Manuel Martín for his help with informatics, and the help of Carmen Ibáñez with the translation of the manuscript. A. P. thanks M. J. de Oliveira for useful observations.

-
- | | |
|--|---|
| <p>[1] P. G. Benedetti, <i>Metastable Liquids</i>, Princeton University Press, Princeton, NJ, 1997.</p> <p>[2] P. G. Benedetti, F. H. Stillinger, <i>Nature</i> 410 267 (2001).</p> <p>[3] J. Jäckle, <i>Rep. Prog. Phys.</i>, 108 171 (1986).</p> <p>[4] P. A. Rikvold and B. M. Gorman, <i>cond-mat/9407027v1</i>, 1994, and references therein.</p> <p>[5] Kauzmann, W., <i>Chem. Rev.</i> 43 219 (1948).</p> <p>[6] K. Binder, <i>Rep. Prog. Phys.</i> 50 783 (1987), and references therein.</p> <p>[7] See references on: J. Biroli and J. Kurchan, <i>Phys. Rev. E</i>, 64, 016101 (2001).</p> | <p>[8] K. Binder, <i>Phys. Rev. B</i> 8 3423 (1973).</p> <p>[9] J. S. Langer, <i>Phys. Rev. Lett.</i> 21 973 (1968).</p> <p>[10] J. S. Langer, <i>An introduction to the kinetics of first-order phase transitions</i>, in <i>Solids far from equilibrium</i>, Ed. by C. Godrèche, Cambridge University Press, 1992.</p> <p>[11] O. Penrose, <i>J. Stat. Phys.</i> 78 267 (1995).</p> <p>[12] J. S. Langer, <i>Ann. Phys.</i> 41 109 (1967).</p> <p>[13] K. Binder and E. Stoll, <i>Phys. Rev. Lett.</i> 31 47 (1973); K. Binder and H. Müller-Krumbhaar, <i>Phys. Rev. B</i> 9 2328 (1974), and references therein.</p> <p>[14] See reference (7) of [11].</p> |
|--|---|

- [15] See references on chapter 6 of [4].
- [16] J. L. Meunier, A. Morel, *Eur. Phys. J. B* **13** 341 (2000).
- [17] F. Y. Wu, *Rev. Mod. Phys.* **54** 235 (1982).
- [18] S. B. Rutkevich, *cond-mat/0201128* (2002).
- [19] H. Arkin, T. Tcelik, *Int. J. Phys. C* **11** 1313 (2000).
- [20] H. Arkin, T. Tcelik, B. A. Berg, H. Meyer-Ortmanns, *Int. J. Phys. C* **10** 1261 (1999).
- [21] B. A. Berg, Urs M. Heller, H. Meyer-Ortmanns, and A. Velytsky *Phys. Rev. D* **69** 034501 (2004).
- [22] A. Velytsky, B. Berg, Urs M. Heller, *Nucl. Phys. B (Proc. Suppl.)* **119** 861 (2003).
- [23] S. Gupta, *hep-lat/9310001v1* (1993).
- [24] E. Ferrero, “Trabajo Especial de Licenciatura”, Universidad Nacional de Córdoba, Argentina (2005).
- [25] R. J. Baxter, *J. Phys. C* **6** L445 (1973).
- [26] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller and E. Teller, *J. Chem. Phys.* **21** 1087 (1953).
- [27] A. Cavagna, I. Giardina, T. S. Grigera, *J. Chem. Phys.* **118** 6974 (2003); A. Cavagna, A. Attanasi and J. Lorenzana, *Phys. Rev. Lett.* **95** 115702 (2005).
- [28] M. J. de Oliveira, A. Petri, T. Tomé, *Europhys. Lett.* **65** 20 (2004); M. J. de Oliveira, A. Petri and T. Tomé, *Physica A* **342** (1-2), 97-103 (2004); A. Petri, *Braz. J. Phys* **33** 521 (2003).
- [29] M. Ibáñez, E. E. Ferrero, S. A. Cannas, V. Loreto, A. Petri, *Eur. Phys. J.-special topics*, **143** 173 (2007). *cond-mat/0610039*.
- [30] P. Hurtado, P. L. Garrido and J. Marro, *Physical Review E* **70** 021101 (2004).
- [31] P. A. Rikvold, H. Tomita, S. Miyashita, S. W. Sides, *Phys. Rev. E* **49** 5080 (1994).