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Weak first order transitions. The two-dimensional Potts model

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We study the two-dimensional Potts model to learn about the pseudocritical behavior observed in some first order transitions. This behavior can be explained by the presence of a second order-like transition point in the metastable region. We calculate the position of this point and measure its *critical* exponents.

First order phase transitions exhibit a wide variety of behaviors. Some of them do not show any pretransitional effect, the transition occurs abruptly and the discontinuities in thermodynamic quantities at the transition are comparable to the overall change in the whole critical region. In other – weak – cases pretransitional effects take place, which can also be very significant: everything goes like if a second order transition which would occur at a certain coupling β^* is preempted from a first order one at a beta $\beta_c \leqslant \beta^*$.

Thus, a weak first order transition behaves like a second order one, near, but not too near, the critical point. For instance, the inverse correlation length should obey the law

$$\xi^{-1}=A(\beta^*-\beta)^{\nu^*}, \tag{1}$$

where β^* and ν^* can be thought of as the coupling and critical exponent of the virtual second order transition point in the metastable region.

Liquid crystals offer a wide sample of behaviors of this kind; the quantity $\beta^*-\beta_c$ has been measured with great accuracy in many real experiments and tested in numerical simulation [1]. A phenomenological theory à la Landau developed by de Gennes [1] provides a satisfactory description of the phenomenon.

Numerical simulations suggest an analogous behavior in several gauge (four dimensional Z_2 theory [2], pure QCD at finite temperature [3]) and spin systems (3-states three-dimensional Potts model [4,5], two-dimensional Potts model [6]). β^* has been actually observed making use of a wide range of techniques, from renormalization group (RG) [6] to the analysis observation of the important precursor effects in the pseudocritical region [3].

This paper, and a forthcoming one [7], aims to clarify the relationship between the various approaches and to provide more precise measurements.

The appealing idea is that the above depicted behavior is a general scheme for weak first order transitions, the second order transition being recovered when $\beta^*\to\beta_c$, the more usual, strong first order one, when $(\beta^*-\beta_c)\gg 1$. In the intermediate region the

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strength of the transition, as measured for instance by the ratio of the discontinuity in the internal energy to the sum of the energy in the ordered and disordered phases, should increase with $\beta^* - \beta_c$.

In this paper we present a study of the two-dimensional q-states Potts model [8] whose action is

$$S = -\beta \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j} , \quad (2)$$

where $\sigma_i = 1, ..., q$, and $\sum_{\langle ij \rangle}$ is extended to all pairs of first neighbor spins.

This simple model presents a ferromagnetic phase transition at every value of q. Many of its properties are analytically known, including the critical coupling and the latent heat [9]. The later turns out to be an increasing function of q, vanishing for $q \leqslant 4$. The transition is thus second order for $q \leqslant 4$ and first order for $q \geqslant 5$, with intensity increasing with q. So the Potts model for $q \geqslant 5$ is an excellent case study of the relationship between the properties of a weak first order phase transition and the second order transition point β^*. Our primary aim is the study of the properties of β^*. First, let us briefly recall the numerical techniques in use to locate an ordinary second order point; they roughly fit in two main categories.

The first one is based on measurements of quantities which show true divergence at the critical point in the infinite volume limit. It is not possible to observe divergence in a finite lattice, but definitely it is possible to measure quantities, like the susceptibility or the correlation length, which would diverge at the second order point but are finite around it. The critical coupling is then obtained by extrapolating the results according to a power law behavior.

The second technique is based on the direct observation of the way in which discontinuities are built up right at the critical point: RG methods, finite size scaling analysis, or a combination of them can be used for this purpose.

Both of the previous approaches can be generalized to the case of interest. In the first case, the generalization is in principle straightforward. For the second approach some extra care is needed: to get β^* we have to work inside the metastable region (which would be very interesting in itself), where the separation between true physics and lattice artifacts is even more difficult from a numerical point of view.

We can discuss the properties of the transition using a simple non-convex effective potential formalism. (Notice that this potential transforms into a physical convex effective potential by taking the convex hull [10]). Let us consider a potential $\phi^\beta(E) \equiv -\log P^\beta(E)$ where E is the total energy and $P^\beta(E)$ the probability density of finding a configuration of energy E at a given β.

Near β_c, $\phi^\beta(E)$ has two local minima at $E_1(\beta)$ and $E_2(\beta)$. The first order point β_c is defined by the condition $\phi^{\beta_c}(E_1) = \phi^{\beta_c}(E_2)$. For β slightly larger than β_c, there will be only an absolute minimum at $E_2(\beta)$, being $E_1(\beta)$ ($< E_2(\beta)$) a local minimum related with metastable states. For β big enough the minimum at E_1 becomes an inflexion point (spinodal point), and the metastability disappears. This coupling has to be identified [1] with β^*, which is thus fixed by the condition

$$\left.\frac{d^2\phi^{\beta^*}}{dE^2}\right|_{E=E_1(\beta^*)=E^*} = 0 . \quad (3)$$

So

$$\phi^{\beta^*}(E) = a_0 + a_3(E-E^*)^3 + \ldots . \quad (4)$$

Using the relation $P^{\beta'}(E) = P^\beta(E)e^{-(\beta'-\beta)E}$ we find that for β near β^*, $\phi^\beta(E) = a_0 + a_3(E-E^*)^3 + (\beta-\beta^*)E + \ldots$ has a local minimum located at

$$E_1(\beta) = E^* + \sqrt{\frac{\beta^*-\beta}{3a_3}} , \quad (5)$$

and the specific heat C_v reads

$$\frac{1}{C_v} \sim \frac{d^2\phi^\beta}{dE^2} \approx 2\sqrt{3a_3}\,(\beta^*-\beta)^{1/2} . \quad (6)$$

We conclude that the system behaves as if it had a second order transition at β^* with a critical exponent

$$\alpha^* = \tfrac{1}{2} . \quad (7)$$

An equivalent procedure can be followed for the potential depending on the total magnetization $\phi^\beta(M)$. Now, the disordered metastable minimum is always at $M=0$ and we can write

$$\phi^\beta(M) = b_0(\beta) + b_2(\beta)M^2 + \ldots . \quad (8)$$

At β^*, b_2 must become zero. By supposing an analytical behavior of b_2 near β^* we obtain for the magnetic susceptibility

$$\frac{1}{\chi} \sim \left(\frac{d^2\phi^{\beta}}{M^2}\right)_{M=0}$$

$$= 2b_2(\beta) \sim (\beta^* - \beta) + O((\beta^* - \beta)^2) , \quad (9)$$

therefore the apparent γ critical exponent is

$$\gamma^* = 1 . \quad (10)$$

It is not possible to use a similar approach to obtain other critical exponents. By using the relation $\gamma = \nu(2-\eta)$ obtained from the fluctuation–dissipation theorem and supposing that the exponent η, related with an anomalous dimension, is zero, we may conclude that $\nu = \frac{1}{2}$ (notice that $\eta = 0$, $\nu = \frac{1}{2}$ are the classical exponents). $D=3$ seems to be the critical dimension where the scaling relation $\alpha = 2 - \nu D$ also holds. The behavior observed in some three-dimensional models [5,3] is in agreement with $\nu = \frac{1}{2}$. In $D=2$ the scaling relation $\alpha = 2 - \nu D$ is violated, since it would imply $\nu = \frac{3}{4}$ ($\eta = \frac{2}{3}$) what we shall see is also excluded by our Monte Carlo (MC) data.

Analogously, there is a pseudocritical point at $\beta^{**} < \beta_c$, related with the ordered metastable states. A similar derivation shows that there must be a pseudocritical behavior with $\alpha^{**} = \frac{1}{2}$, but in this case, the exponent for the susceptibility cannot be computed directly.

It would be very interesting to check the previous results with a numerical simulation in the metastable region. Unfortunately this is not easy since the inhomogeneous configurations can obscure the physics of the transition. This problem is related with the convexity of the physical effective potential in the thermodynamical limit [11]. Further discussion will be presented elsewhere [7].

In this letter we will limit ourselves to the results obtained working at a safe distance from the critical points in order to avoid the inhomogeneous configurations.

We have worked mainly with the 7-states Potts model, however we have done some runs in the 10-states model to see the trend in $\beta_c - \beta^*$. For our MC simulation we have used a standard heat bath method for generating configurations. We worked on lattices whose sizes range from 32×32 to 128×128 at different values of β. The number of MC sweeps has been between one and two millions. We have run the code on transputer networks as well as on VAX computers.

At each measure sweep we stored the total energy, the magnetization, and correlation function between lines. In the analysis of data we have used the spectral density method [12], however we put special attention to direct simulations (without extrapolating to different β values) to have a safer estimation of the errors. The statistical errors have been computed with the jack-knife method using about 10 bin of data.

The correlation length is computed measuring the correlation function between the magnetization of parallel lines of spins. In a $L \times L$ lattice

$$C(d) \equiv \frac{1}{2L^3}\left(\sum_x \boldsymbol{M}_{x+d}\boldsymbol{M}_x + \sum_y \boldsymbol{M}_{y+d}\boldsymbol{M}_y\right) - \frac{1}{q} , \quad (11)$$

with

$$\boldsymbol{M}_x = \sum_y \boldsymbol{\mu}_{xy} , \quad (12)$$

where $\boldsymbol{\mu}_{xy}$ is the magnetization q-vector of the spin at the point (x, y) (for a spin in state $\sigma \in \{1, \ldots, q\}$ the nth component of $\boldsymbol{\mu}$ is $\delta_{n\sigma}$). The correlation length ξ is computed fitting $C(d)$ to the function $\cosh((d - \frac{1}{2}L)\xi^{-1})$.

A reliable measure of the correlation length or specific heat requires all the configurations to be homogeneous (this amounts to say that we want true $V \to \infty$ estimates). We shall work at β *far enough* from β_c, where the appearance of inhomogeneities is strongly suppressed, then we shall extrapolate to the critical point (see fig. 1).

We have run in several lattice sizes and analyzed the asymptotic (large L) behavior. All the results reported in this letter have been checked to be free of finite size effects. See also ref. [13] for a recent, very careful discussion of finite size effects in Potts model.

We have focused our attention in the measure of the correlation length. We have confidence that the systematic errors due to finite size effects are smaller than the statistical ones. As previously noted, another source of systematic error is the appearance of inhomogeneities. We have not found evidence of that for $\beta \leq 1.292$ after several millions of MC sweeps.

In a first stage we compute the exponent ν^* as well as the critical point β^* by a three parameter fit of the correlation length to the function $A(\beta - \beta^*)^{-\nu^*}$. Our results for ν^* are

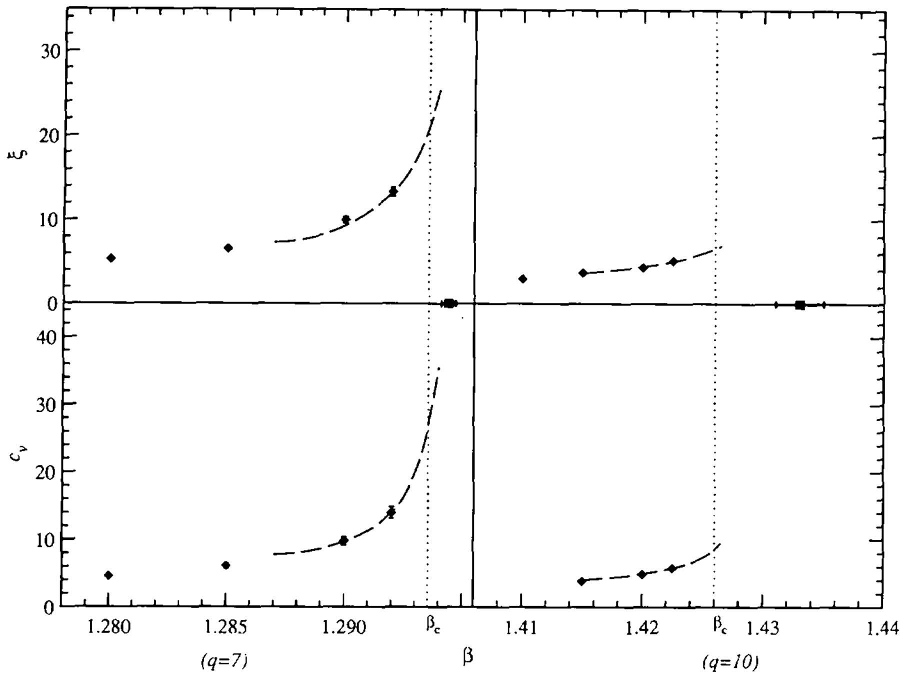

Fig. 1. Specific heat $c_v=(\langle E^2\rangle-\langle E\rangle^2)/V$ (lower side) and correlation length ξ (upper side) for the 7-states (left) and 10-states (right) Potts model. The dashed lines have been obtained with the spectral density method from the rightmost point data.

$$\nu^*=0.53(8)\,, \tag{13}$$

$$\beta^*=1.2945(9)\,. \tag{14}$$

This value is incompatible with the scaling prediction 0.75 and in accordance with the guess of the classical $\nu=\frac{1}{2}$.

Unfortunately it is not possible to give a precise value for β^* from the three-parameter fit, although it is clear that $\beta^*>\beta_c$. Notice that there is a shift of β_c due to finite size effects that decreases as L^{-2}. We have measured this shift extrapolating the $\beta_c(L)$ obtained in smaller lattices to the value $\beta_c(L=128)=1.2933$.

However, assuming $\nu^*=\frac{1}{2}$ we can obtain a better estimation of β^*. In fig. 2 we plot the ξ^{-1} values squared, as a function of β. The linear behavior is very clear. We have computed β^* both by fitting the points obtained directly in the numerical simulation and using the spectral density method at the point $\beta=1.292$ with a full agreement. Our final result is

$$\beta^*=1.2944(3)\,. \tag{15}$$

Another interesting quantity is the maximum correlation length (at β_c). We have obtained

$$\xi_{max}=24(5)\,, \tag{16}$$

to be compared with the estimation 30 of ref. [13] based on an extrapolation from $q=10$ results.

The transition in the $q=7$ model is so weak that it is very difficult to measure the maximum correlation length or the value of β^*. We have needed large lattice sizes as well as long MC simulation due to *critical* slowing down.

For a stronger transition it is expected that the maximum correlation length will be smaller, and β^* is farther from β_c, and consequently easier to compute. Nevertheless, the second order-like behavior will not be so clear.

We have also measured the correlation length for $q=10$ in lattices up to $L=96$. The results are summarized in fig. 3. Although the linear behavior of $1/\xi^2$ versus β is not as precise as in the $q=7$ case, it is still rather clear.

The maximum correlation length is found to be

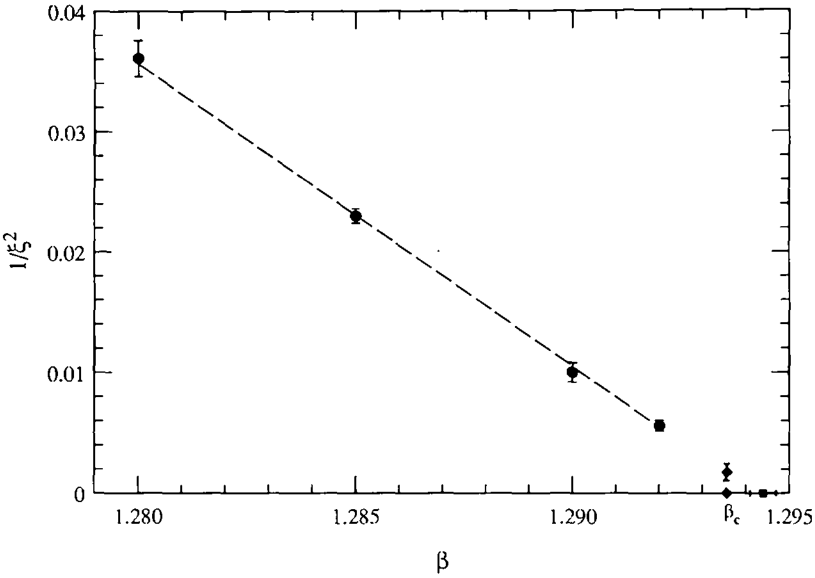

Fig. 2. Inverse correlation length squared as a function of β for $q=7$. We also plot our computed values for ξ_{max} (rhomb) and β^* (square)

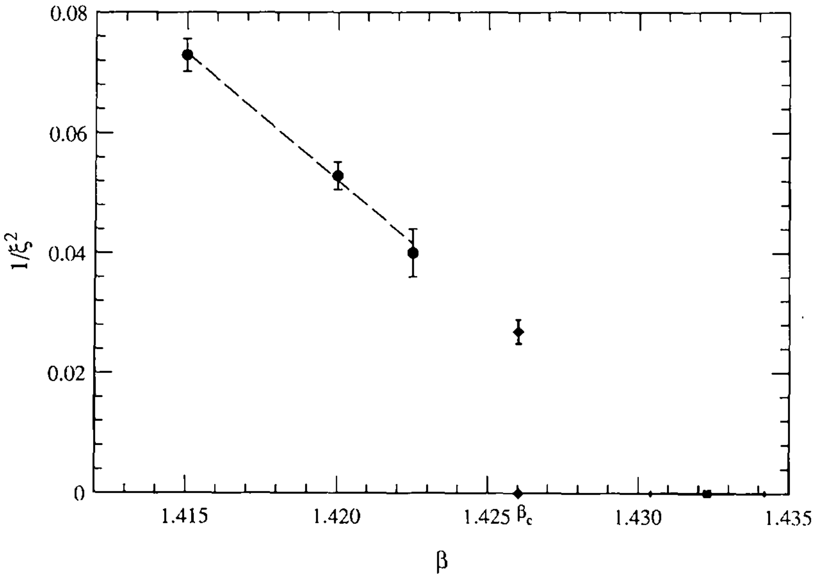

Fig. 3. Inverse correlation length squared as a function of β for $q=10$, and ξ_{max} (rhomb) and β^* (square) values.

$$\xi_{max}=6.1(5)\,, \tag{17}$$

to be compared with the estimation $\xi=5.9(7)$ of ref. [14].

The computed value of β^* using the correlation length data and fixing ν^* to $\frac{1}{2}$ is

$$\beta^*=1.433(2)\,, \tag{18}$$

while $\beta_c=1.4260$ and its shift due to finite size effects gives $\beta_c(L=96)=1.4254$.

We have analyzed the properties of the weak first order ferromagnetic transition of the two-dimensional Potts model obtaining a good description of its behavior considering a second order-like transition in the metastable region. We think that the picture presented in this paper for the 2D Potts model is general for weak first order transitions, behaving as a pseudouniversality, what is supported by the results obtained in other models. We find critical exponents in good agreement with their mean field values, what has been observed experimentally in a wide variety of systems. We remark that the measure of the apparent critical exponents can be useful to distinguish between a weak first order transition and a true second order one.

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