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Comments on the phase diagram of the three and four-state chiral Potts model

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Abstract The phase diagrams of the isotropic three and four-state chiral Potts model are studied using exact results and Monte-Carlo simulations performed on twisted square lattices with different sizes (up to 64x64 for the three-state Potts model). A floating phase starting immediatly from the critica1 ferromagnetic standard scalar Potts model seems to occur. Important finite size effects occur as expected. The phase diagram is seen to be even more involved in the case of the four-state chiral Potts model.

1. Introduction

Two years ago Au-Yang et al obtained integrable cases for the N-state chiral Potts model[1,2] which happened to be the first solvable model with genus greater than one parametrization (see for instance refs.3,4). This breakthrough has renewed the interest in those models that generalize an important model of two-dimensional statistical mechanics, the (standard) scalar Potts model (for a review

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see ref. 5) and exhibit interesting physical properties and rich phase diagrams (commensurate-incommensurate transitions, floating phases (for a review see for instance ref. 6), Lifshitz points[7], possible occurence of a new chiral universality class[S]. Many subcases of this niodel have been considered with different names: clock models, helical models... Recause it is known to exhibit (in two dimensions) an incommensurate floating phase (i.e. a phase with algebraically decaying order parameter correlations) the three-state chiral clock model (CC3) introduced by Huse and Ostlund[10] has attracted great attention. The literature on these subjects is very large. Among many one can read for instance Selke and Yeomans[11], Everts and Röder[12] and Everts[13], von Gehlen and Rittenberg[14], den Nijs[15], Vexan et al[16], Albertini et al[17,18]...

This paper is divided into two different parts: the analysis of the exact results and symmetries of the anisotropic N-state chiral Potts model and the results of simulations performed only on the isotropic three-state chiral Potts model. Of course all the ideas developed here are not restricted to isotropic models: we restrict ourselves to isotropic models for reasons of clarity and because many results can be found in the literature on different kinds of anisotropic models[19], on very anisotropic models (strong coupling limits) and on low temperature properties of the chiral model[10]. On the other hand the (finite temperature) isotropic chiral Potts models have not been so extensively studied.

The purpose here is to shed some light on the relations between the notions of criticality, integrability and self-duality in models like the chiral Potts model for which many partial results are available and for which these notions no longer coincide. We try also to understand the role played by the integrability curve of Au-Yang et al in the phase diagram of the model.

2. Symmetries and exact results for the N-state chiral Potts rnodel

The partition function of the anisotropic N-state chiral Potts model on a square lattice reads:

$$Z = \sum \prod w(\sigma_i - \sigma_j) \prod \bar{w}(\sigma_j - \sigma_k) \tag{1}$$

where the first (resp.second) product is taken over all oriented horizontal (resp. vertical) bonds of the square lattice. The spins belong to Z_N and the two sets of parameters consist of N homogeneous variables w(O),$w(1), ... w(N-1)$ and $\bar{w}(0)$, w$(1),..\bar{w}(N-1)$.The anisotropic model has some obvious symmetries on the square lattice that amount to performing simple transformations on the dummy variables σ_i and correspond to the following permutations of the $w(i)$'s

$$C : w(0) \to w(1) \to ...... \to w(N-1) \to w(0) \tag{2a}$$

and

$$S : w(i) \leftrightarrow w(N-i) \tag{2b}$$

and of course similar transformations on the $w(i)$'s. S corresponds to spin reversal on the spins and the N-cycle C amounts to performing a translation on σ_j but not σ_i. C and S generate a dihedral group: one has for instance the following relation between C and $S : (CS)^2 = 1$.

In the thermodynamic limit one must also take into account the symmetry of permutation of the horizontal and vertical homogeneous parameters $w(i)$ and w(i).

A duality symmetry exists for this model (see for instance ref. 20). it corresponds to the following linear transformation:

$$D : \hat{w}(n) = \sum \omega^{np} \ w(p) \tag{3}$$

where w is an N^{th} root of unity, $\omega^N = 1$ (and of course similar transformations on the $\bar{w}(i)$'s). ***For every value of N, D*** is a transformation of order four, D^2 being a transformation identical to S.

The new results of Au-Yang et al[1] and Baxter et al[3] show that a star-triangle relation exists in the model provided certain (homogeneous) relations between the

$w(i)$'s and $\bar{w}(i)$'s are satisfied: a first set of conditions comes from the compatibility conditions for an overdetermined homogeneous system to have non-trivial solutions. These conditions correspond to the vanishing condition of determinants and occur only for N > 4. They are actually conditions bearing separately on the two horizontal and vertical parameter spaces:

$$F_\alpha\left(w(0), w(1), ...w(N-1)\right) = 0 \tag{4a}$$

$$F_\alpha\left(\bar{w}(0), \bar{w}(1), ...\bar{w}(N-1)\right) = 0 \tag{4b}$$

and $\alpha = 1, ...N-3$.

The symmetries of the anisotropic chiral Potts model (generated by the inversion relation, permutation of horizontal and vertical couplings, duality...) are in general an infinite set of (birational) transformations on the parameter space of the model[21]. It has been noticed that the previous solutions of the Yang-Baxter equations correspond precisely to the case where this set degenerates into a finite set. Moreover this finite set of symmetries is deeply related to the set of automorphisms of the algebraic curves of genus greater than one that occur in the parametrization of the solutions: these results are particularly obvious when one introduces well-suited variables to analyze this set of symmetries[22].

To this set of determinantal equations one must also add one equation that mixes the horizontal and vertical parameters:

$$R(w(0), w(1), ...w(N-1)R(\bar{w}(0), \bar{w}(1), ...\bar{w}(N-1)) = 1 \tag{5}$$

where R is a rational expression of the $w(i)$'s[22].

From now on we concentrate on the N = 3 and N = 4 isotropic chiral Potts models.

Ia) - The three-state chiral Potts model

For the N = 3 model there is no determinant condition like (4a,b) and eq.(5) reads:

$$w(0)w(1)w(2)^4 + w(1)w(2)w(0)^4 + w(0)w(2)w(1)^4 + 3w(0)^2w(1)^2w(2)^2 - 2w(0)^3w(1)^3 - 2w(1)^3w(2)^3 - 2w(0)^3w(2)^3 = 0 \tag{6}$$

This integrability curve is actually invariant under the other symmetries of the model C, S, D.

We pay particular attention to the following sets of points of the phase diagram:

-the line *globally* invariant under the duality transformation (self-dual line):

$$\sqrt{3}w(0) = w(0) + w(1) + w(2) \tag{7}$$

(there is another self-dual line which is not in the physical domain: $\sqrt{3}w(0) = w(0) + w(1) + w(2)$).

-the line where the model reduces to the standard scalar Potts model $w(1) = w(2)$ and their transform by C and C^2. The critica1 point of the ferromagnetic three-state standard scalar Potts model (the intersection of the standard scalar condition $(w(1) = w(2))$ and of the self-dual line (7): point H of fig. i a also belongs to curve (6). Because of the symmetries (2a,b) and because the $w(i)$ are homogeneous variables, it is convenient to introduce the two variables a and b:

$$a = (w(0) - 2w(1) + w(2))/\sqrt{6}(w(0) + w(1) + w(2))$$

$$b = (w(0) - w(2))/\sqrt{2}(w(0) + w(1) + w(2)) \tag{8}$$

In these new variables (a,b) the physical domain is then restricted to the triangle (ABC) drawn on fig. 1a. The boundaries of the physical domain ($w(0) = 0$ or $w(1) = 0$ or $w(2) = 0$) are the edges of the triangle and also correspond to limits where the chiral model can be mapped (in the thermodynamic limit) onto a six vertex model in direct fields[23]. The self-dual line (7), the standard scalar Potts line, their transforms by C and C^2 and curve (6) have also been drawn on **fig.** 1a. Due to the symmetries (2a,b) one can restrict the study of the phase diagram to the (physical) triangle AOD. The two edges (AO),(OD) of this triangle correspond respectively to the isotropic three-state ferromagnetic (resp. antiferromagnetic) standard scalar Potts model ($w(0) > w(1) = w(2)$, resp. $w(1) > w(0) = w(2)$). Point D is the completely ordered limit of the antiferromagnetic scalar Potts model. Point A ($w(1) = w(2) = 0$) corresponds to a completely ordered state, while point O corresponds to the completely disordered one (no interactions between the spins).

As the model can be mapped, in the $w(1) = 0$ limit, onto a six vertex model in direct fields[24,25], one can actually locate a critical point on this edge of the triangle (ice point) for $w(0)/2w(2) = 1$) (see for instance inequalities (355a) on page 436 of Lieb and Wu[26]). Note that this point (G in figure 1a,b) is not on the self-dual line (7) (point E). Point H corresponds to the critical ferromagnetic three-state standard scalar Potts model. Points G and H are actually critical points of a very different nature: *is there a critical curve conneeting G and H* ? Using a result of Kardar (ref. 23, eq. (14)) one can argue that there should exist, close to point H, a critical curve orthogonal to the standard scalar Potts line (AO) at point H.

Criticality, integrability and self-duality are notions having often some overlap for two-dimensional models. The Ashkin-Teller models, the Z_n models[27,28] are some examples. The scalar Potts model is a typical example for which a star-triangle relation exists precisely when the model is critical[29]: this can be understood very roughly as saying that these conditions must correspond to enhanced symmetries of the model. So the first question addressed in the simulations of paragraph II concerns the criticality of the model on condition (6) and also (7).

Ib) - Four-state chiral Potts model

Let us consider now the four-state chiral Potts model. The analysis performed for the three-state chiral Potts model can be generalized mutatis-mutandis: the triangle of fig. 1a is replaced by a tetrahedron $M_0 M_1 M_2 M_3$, a point M in this

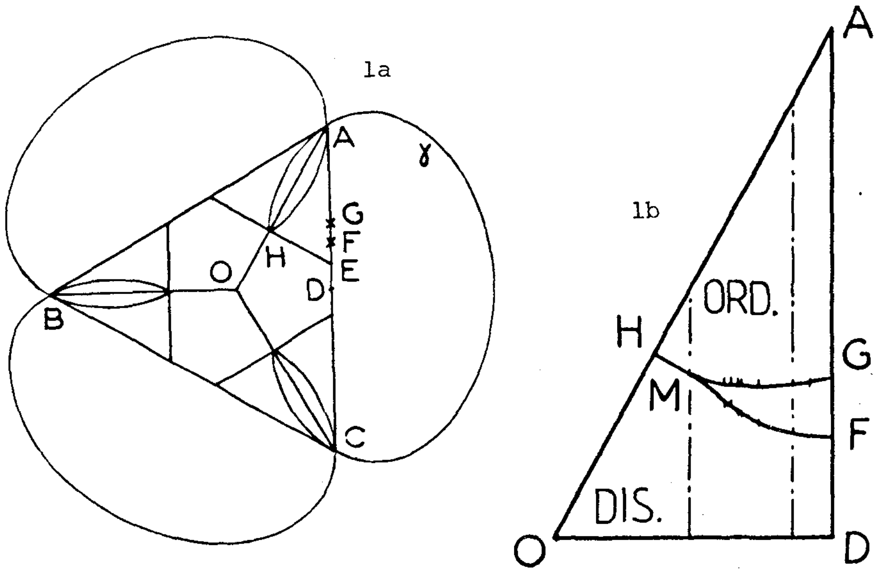

Fig. 1a - Phase diagram of the three-state chiral Potts model in the (a,b)-plane where a and b are defined by (6). The inside of the triangle (ABC) corresponds to the physical domain. On line (AO) the chiral model reduces to the standard scalar Potts model. Line (HE) is the.seld-dual line (5). Curve 7 corresponds to the star-triangle condition (4). Fig. 1b - Region (OAD) of the physical triangle. Region (OHFD) corresponds to the disordered phase while region (HAG) corresponds to an ordered one. Region (GMF) could be a new phase. The broken lines correspond to the sweeps for a=0.20 and a=0.35.

parameter space being associated to the homogeneous parameters $w(i)$ in the following way:

$$\sum_{i=0}^{3} w(i).\,\overrightarrow{MM_i} = \vec{0}$$

One has interesting exact subcases for this model:
$w(i) = w(i+1) = 0$ for $i = 0$ (or $i = 1$ or 2 or 3) correspond again to a six vertex model in direct (and equal) fields[24,25], while $w(0) = w(2) = 0$ or $w(1) = w(3) = 0$ correspond to a mapping onto an Ising (free-fermion) model. This means that one is able to locate critical points on the six edges M_iM_j of the tetrahedron: eight corresponding to the critical points of the six vertex model in direct fields

and four to the critica1 point of the two-dimensional Ising model (see **fig.** 2a). The symmetric Ashkin-Teller rnodel is another interesting subcase of the four-state chiral Potts model[30,31,32]. To make this clear let us consider the four-state Potts spin as two Ising spins σ_i and τ_i. With this notatíon, the Boltzmann weight corresponding to the interactiori between two nearest neighbour spins (σ_i, τ_i) and (σ_j, τ_j) reads:

$$\{(w(0)w(2)w(1)w(3))^{1/4}\} \cdot \{(w(0)/w(2))^{1/4}\}^{\sigma_i \cdot \sigma_j \cdot \tau_i \cdot \tau_j + \tau_i \cdot \tau_j}$$
$$\times \{(w(0)w(2)/w(1)w(3))^{1/4}\}^{\sigma_i \cdot \sigma_j} \cdot \{(w(3)/w(1))^{1/4}\}^{(\sigma_i - \sigma_j) \cdot \tau_i \cdot \tau_j} \qquad (9)$$

Let us note that the spin reversal symmetry $(\sigma_i, \sigma_j) \rightarrow (-\sigma_i, -\sigma_j)$ corresponds to the transposition $w(1) \leftrightarrow w(3)$, while the spin reversal symmetry $\tau_i \rightarrow -\tau_j$ corresponds to the symmetry $w(1) \leftrightarrow w(3)$ and $w(0) \leftrightarrow w(2)$. The 4-cycle $w(0) \rightarrow w(1) \rightarrow w(2) \rightarrow w(3) \rightarrow w(0)$ corresponds to changing r, to $-\tau_j\sigma_j$, σ_j to $-\sigma_j$ and leaving τ_i and σ_i invariant. From eq.(9) it is staightforward to see that there exist other two-dimensional Ising (free-fermion) limits: the line of equations $w(1) = w(3)$ and $w(0) = w(2)$ and the curves of equations $w(1)w(3) = w(0)w(2)$ and $w(1) = w(3)$ or $w(0) = w(2)$. For $w(1) = w(3)$, the model obviously reduces to a symmetric Ashkin-Teller model (it corresponds to the fact that the model is no longer chiral). This is also the case for $w(0) = w(2)$ (change τ_j to $-\tau_j\sigma_j$, σ_j to $-\sigma_j$ and keep τ_i and σ_i invariant). In this (symmetric) Ashkin-Teller limit, the phase diagram of the model is well-known[33]. In particular, one recalls the existence of a critica1 self-dual line[s4] in the plane $w(1) = w(3)$ (or $w(0) = w(2)$) of equation $w(0) = w(1) + w(2) + w(3)$ (bowever, it is very unlikely that the self-dual plane $w(0) = w(1) + w(2) + w(3)$ could be a critica1 plane outside the Ashkin-Teller conditions $w(1) = w(3)$ or $w(0) = w(2)$). From these different exact subcases, one remarks that the phase diagram of the four-state chiral Potts model is a much more involved phase diagram than the one of the three-state model. The critical manifolds contain quite different critica1 points like points S_i (critica1 points of a six vertex model in direct fields) and like points I_i (critica1points of a free-fermion

Ising model) (see fig. 2a). These ideas can of course be generalized to higher values of N: the corresponding phase diagrams will depend very much on whether N is a prime number or not. The critica1 behaviour of these models for any N also indicates a rather involved situation: along the standard scalar Potts varieties the transition is first order for N > 4 and along the integrability varieties one gets[4] the following value for the exponent α : $a = 1 - 2/N$.

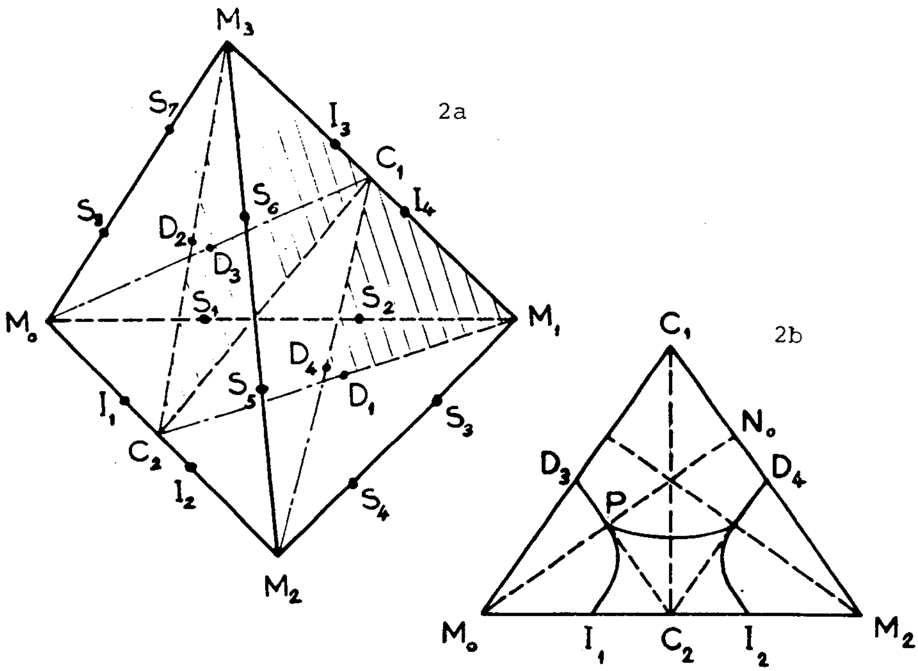

Fig. 2a - Phase diagram of the four-state chiral Potts model. The inside of the tetrahedron $(M_0M_1M_2M_3)$ corresponds to the physical domain. Points $S_1, \ldots S_8$ correspond to critical points of the six vertex model in direct field, $I_1, \ldots I_4$ to the critical points of the two-dimensional Ising model. The $(M_0M_2C_1)$ and $(M_1M_3C_2)$ planes correspond to the (symmetnc) Ashkin-Teller limit of the model. $C_1D_1, C_1D_2, C_2D_3, C_2D_4$ are self-dual lines of the Ashkin-Teller model. Fig. 2b - Phase diagram in the $(M_0M_2C_1)$ Ashkin-Teller plane. The line (M_0N_0) correspond to the standard scalar four-state Potts model. Point P is the (ferromagnetic) critical point of the standard scalar four-state Potts model.

3. Monte-Carlo simulations

Monte-Carlo simulations have been performed on a parallel computer built in the CRTBT which consists of forty-six M68000's working in parallel. This parallel computer allows us to average the results over a rather large nurnber of samples. This analysis has been performed for the three-state *isotropic* chiral Potts model to be able to study large enough samples.

We study $L \times L$ square lattice with helical boundary conditions $L = 4, 8, 16, 32, 64)$. Most of the trajectories in the (AOD) triangle are sweeps in the (a,b)-plane which correspond to keeping constant the value of a and to decreasing b, but trajectories allowing a sirnple use of the fluctuation-dissipation theorem (trajectories with given coupling constants, given chirality...) are also considered. A measure of the relevant quantities (internal energy, fluctuation of the internal energy ...) is performed every ten Monte-Carlo steps (MCS) per spin. For instance in the $L = 64$ (resp. 16) case 5000 MCS per spin are discarded (to therrnalize the system) and 10^8 (resp. 4×10^8) values are averaged. For the $L = 64$ case, for instance, *it* represents 4 x 10^{11} updates and it took three weeks (for a given value of a) on the parallel computer (the total number of updates corresponding to *all* the simulations performed here is 5×10^{12}.)

Different runs along trajectories in the parameter space corresponding to the standard scalar Potts model ((AO) in fig. 1a) have been performed to check the validity of our program. As already mentioned by Barber[35], due to important corrections to scaling, discrepancies in the value of exponent obtained from the finite size scaling analyzis occur but the location of the critica1 point is obtained quite accurately.

To investigate the criticality of the integrability curve (6) and of the self-dual line (7) sweeps for a=0.20, 0.25 and different values of L ($L = 4, 8, 16, 32, 64$) have been perforrned. The results are shown in the insert of figure 4: $c(b)$ presents a maximum which becomes sharper with increasing values of L. The system seems to undergo a second order phase transition between an ordered and a disordered phase as could be remarked inspecting representative spin configurations just above the transition (see fig. 3a). For a=0.20 this breaking takes place through flips of isolated clusters of spins in an ordered phase. The ordered phases correspond to a ferromagnetic state and to helical states[23] (< ...012... >, resp. < ...021... >) for the other ordered phases of the phase diagram (points B and C). One locates quite accurately the critica1 point corresponding to the maximum. ***One notes that the value of*** b ***corresponding to the integrability curve is clearly to be discardes as well as the self-dual value. The "simplicity" arguments which would have identified the critical curve with the self-dual line actually fails.*** Curve (6), if critical for the chiral three-state Potts model, corresponds to a very weak singularity. However one can imagine that the integrability curve (6) has to be a "special" curve in the parameter space. One could think of a connection between this curve and a wetting transition curve (compare, up to the change of variables $(a,b) \rightarrow (\beta J, A)$, the integrability curve (6) (7 in fig. 1a) and the interfacial wetting transition dotted lines of figure 1 of Huse et al[19]. On the other hand these results indicate that the critica1 curve, although different, is located close to the self-dual line near point H. This is in agreement with the previously mentioned result of Kardar that the critica1 curve exists in the neighborhood of point H and has to be orthogonal to the line (AO) at point H.

Monte Carlo simulations were carried out for L = 16 and a = 0.35 in order to follow this transition for larger values of a. The situation is now more involved: c(b) exhibits two maxima (fig. 5). For L = 32 we get then three maxima and for L = 64 six maxima. These results indicate a rather involved phase structure for $a = 0.35$ in a certain range $\{b_{min}, b_{max}\}$ of b: the ***setting of the equilibrium seems to be slower as*** can be verified for trajectories that enable one to get into this new phase and correspond to a given chirality for instance $A = -0.42$ [36]. Such trajectories allow an easy use of the fluctuation-dissipation theorem and therefore one can control the setting of the equilibrium. A difference between the order breaking mechanism of the system appears very clearly comparing the snapshots of the spin configurations of the system for a < 0.2 and for $a > 0.2$. (see fig. 3a,b,c for snapshots for $a = 020$ and $a = 0.35$). In opposition to the $a = 0.20$ situation, clusters of spins organised in walls running diagonally through the whole lattice occur for $a = 0.35$. This is reminiscent of a floating phase[6]. Of course everything must be very sensitive to the choice of boundary conditions: with our choice of boundary conditions the number of walls must be divisible by three. The maximum of $c(b)$ occur precisely when the number of walls increases by three. Note that the run performed for L = 16 already gave a reliable estimation of the extension of this "new phase". Sweeps for different values of a (0.26, 0.265, 0.270, 0.275, 0.30, 0.37) have been carried out for L = 16 to get the extension of this "new phase". These simulations indicate two maxima which trace the location of $\{b_{min}, b_{max}\}$ (fig. 1b).

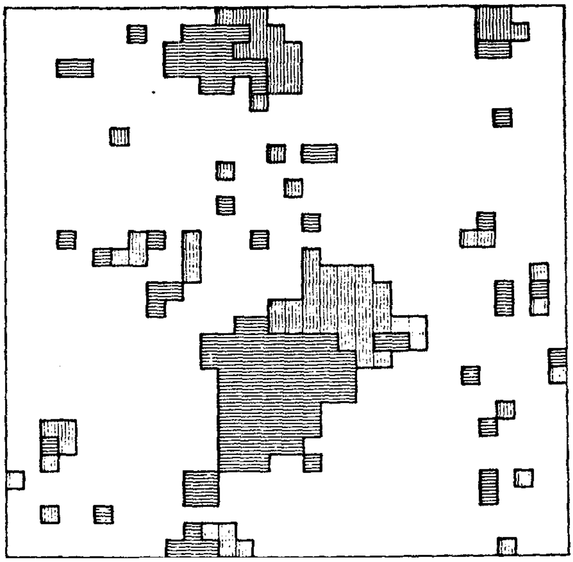

Fig. 3a - Snapshot for a = 0.20 and b = 0.230.

4. Discussion and prospects

The phase diagram of the three-state chiral Potts model has been seen to be a surprisingly rich one and the phase diagram of the four-state chiral Potts model should be even richer. From exact results we have located certain critical points of the isotropic N-state chiral Potts model. For the three-state isotropic chiral

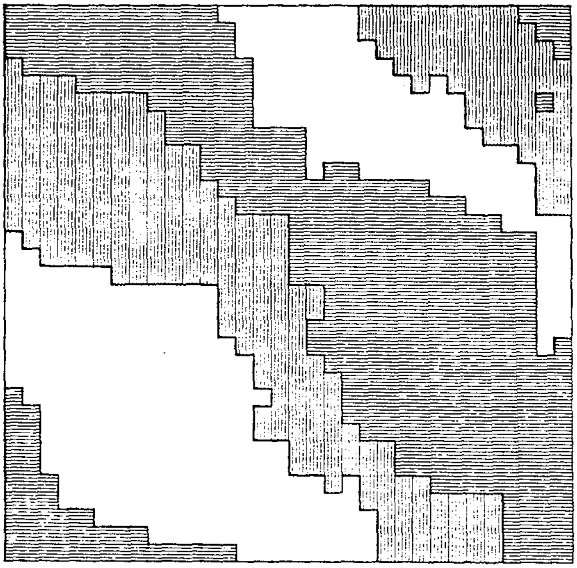

Fig. 3b - Snapshot for a = 0.35 and b = 0.200.

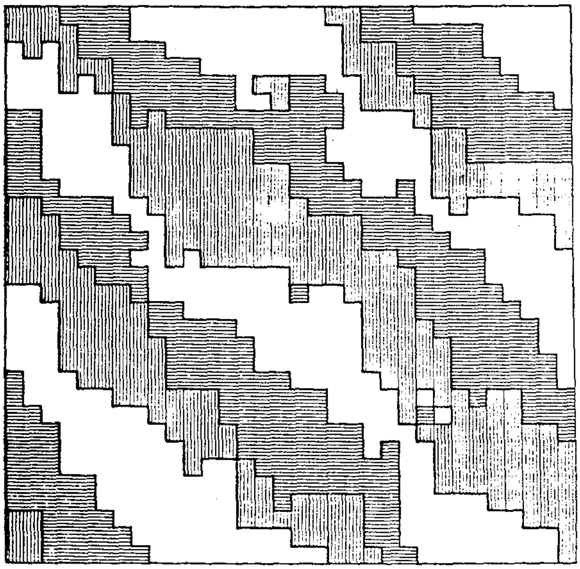

Fig. 3c - Snapshot for a = 0.35 *and* b = 0.185.

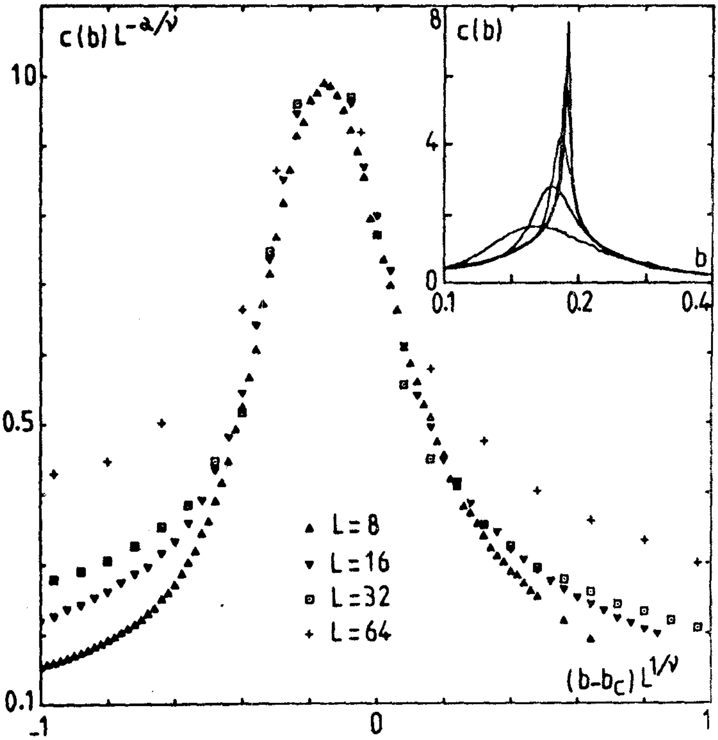

Fig. 4 - Finite size scaling for c(b) for a=0.20 and L=8,16,32,64 with $1/\nu =$ 1 and $\alpha/\nu = 0.5$. The insert shows the original data.

Potts model it has been shown, using Monte-Carlo simulations, that these points are in fact connected by continuous phase boundaries which define, in the phase diagram, ordered and disordered phases and a domain where the phase structure is reminiscent of a floating phase. Critical curve(s) have been located with accuracy for $a < 0.2$. The situation consistent with the evidence obtained here seems to be the following: the critical ferromagnetic standard scalar Potts *point* H *might be in fact a multicritical point, the two critical curves originating at point H being hardly distinguishable near H.* One should recall that Albertini et al[17,18] have been able to see a commensurate-incommensurate transition in the ground state of the

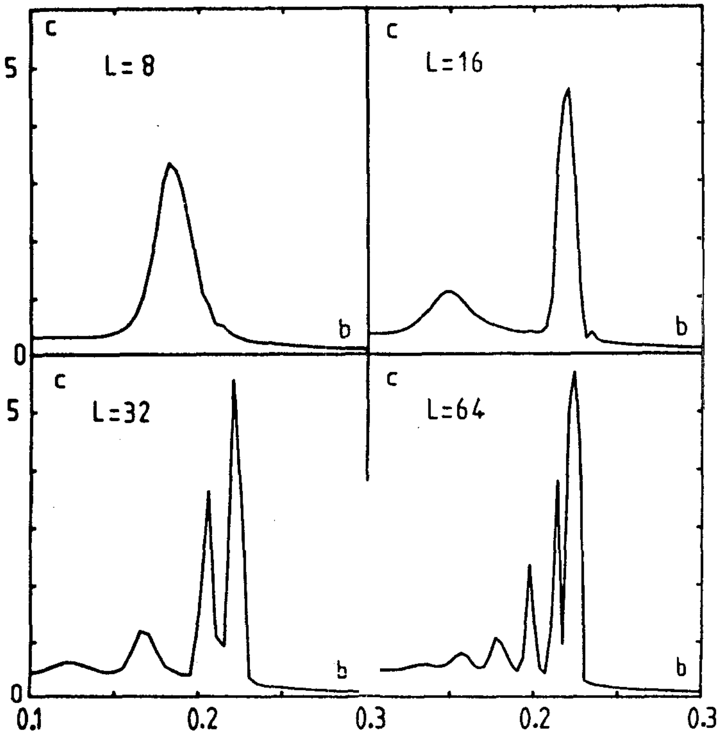

Fig. 5 - c(b) for different values of L for a = 0.35.

superintegrable chiral Potts models and one can compare for example fig. 1b here and fig. 2 of Albertini et al[18] which corresponds to a schematic plot of the phase diagram of the three-state chiral Potts model.

On the other hand a certain ambiguity remains on the localization of point F (see fig. 1b). This ambiguity is difficult to clarify since the local Monte-Carlo algorithm clearly fails in the neighbourhood of (AD)-line. It is not proved that point F is definitely different from point E or even D.

Other studies are necessary to get a better understanding of this intermediate phase. A simulation for a 128×128 lattice and for a given chirality $A = -0.42$ is in progress[36] and seems to confirm the previous analyzis. Simulations have also been performed on anisotropic lattices with similar results. As Monte-Carlo simulations for the four-state for sufficiently large sizes cannot be envisaged reasonably, it would be interesting to perforrn similar simulations on the triangular (resp. honeycomb) three-state isotropic chiral Potts model for which one symmetry (S) still exists but symmetry C does not.

The self-dual line (7) is not critical. The criticality of self-dual lines was natural for Z_n models[27,28] because *these lines are not only globally invariant by duality but each of their points are invariant: this is no longer thc case for chiral models.* Let us emphasize when the critical boundaries are only *globally* invariant by duality that, their algebraicity is often a consequence of an integrability (for instance the identification of the self-dual line with a critical curve should have had its origin in an integrability of the self-dual line but one can actually verify that the star-triangle relation, or any simple generalization of it, is not obviously satisfied when the self-dual condition (7) is satisfied). Finally from a more general point of view, one can expect the integrability curve (6) to be some "special" curve: from the previous simulations one sees that it is included in the ordered phase of the phase diagram (see fig. 1a). What kind of "special" phenomenon can occur in an ordered phase? Presumably only very subtle transitions such as wetting-like transitions.

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Resumo

Os diagramas de fase do modelo de Potts quiral isotrópico com três e quatro estados são estudados, usando resultados exatos e simulações de Monte Carlo realizadas em redes quadradas retorcidas de diferentes tamanhos (até 64×64 para o modelo de Potts de três estados). Parece ocorrer uma fase flutuante começando imediatamente do ponto crítico do modelo de Potts .escalar ferromagnético usual. Como esperado, ocorrem importantes efeitos de tamanho finito. Obtém-se um diagrama de fase ainda mais complexo para o modelo de Potts quual de quatro estados.