J. Phys. A: Math. Gen. **22** (1989) 2577-2585. Printed in the UK

On the phase diagram of the chiral Potts model

J C Anglès d'Auriac†‖, D Hansel‡¶ and J M Maillard§

† Department of Physics and Astrophysics, Rutgers University, 180 College Avenue, New Brunswick, NJ 85500, USA

‡ Racah Institute for Theoretical Physics, Hebrew University, 91904 Jerusalem, Israel

§ Laboratoire de Physique Théorique et Hautes Energies, Tour 16, 4 place Jussieu, 75252 Paris Cedex 05, France

Received 1 December 1988

Abstract. We study the phase diagram of the isotropic three-state chiral Potts model. Monte Carlo simulations performed on twisted square lattices with different sizes up to 64×64 indicate different types of critical curves. In particular, a floating phase seems to occur. Finite-size scaling analyses are performed at some specific critical points. The phase diagram we propose is discussed using exact results.

The N-state chiral Potts model can describe systems that exhibit commensurate-incommensurate transitions (for a review see Selke 1988). Some chiral Potts models have been studied using the Migdal-Kadanoff approach (Huse 1981), Monte Carlo simulations (Selke and Yeomans 1982), free fermion analysis (Ostlund 1981) and transfer matrix calculations (Everts and Röder 1989). Some associated quantum Hamiltonians have also been considered (von Gehlen and Rittenberg 1985, Hoeger *et al* 1985, den Nijs 1988). Recently Au Yang *et al* discovered integrable cases for the N-state chiral Potts model (Au Yang *et al* 1987, McCoy *et al* 1987) which happened to be the first solvable model with genus greater than one parametrisation (see, for instance, Baxter *et al* 1988, Baxter 1988). These breakthroughs renewed interest in these models as they exhibit rich phase diagrams and interesting physical properties.

In this paper we consider the *isotropic* three-state chiral Potts model. On the basis of Monte Carlo simulations we show that the model exhibits a rich phase structure. The locations of the critical boundaries of the different phases is discussed and finite-size scaling analyses are performed. This leads to an estimation of the critical exponents.

The partition function of the isotropic three-state chiral Potts model on a square lattice is

$$Z = \sum_{\{\sigma_i\}} \prod_{\langle ij \rangle} w(\sigma_i - \sigma_j) \prod_{\langle jk \rangle} w(\sigma_j - \sigma_k) \tag{1}$$

the first (second) product concerns all oriented horizontal (vertical) bonds on the square lattice. The spins belong to $\mathbb{Z}_3$ and the parameter set consists of three homogeneous variables $w(0)$, $w(1)$, $w(2)$. The correspondance between these homogeneous variables and more standard ones is simple: $w(n) = \exp\{-\beta J \cos[2\pi/3(n+\Delta)]\}$ where J is the nearest-neighbour coupling constant, Δ is the chirality of the model and β is the inverse of the temperature: $\beta = 1/kT$. However, in our analysis some particular limits of the parameters of the model are useful. In

‖ Permanent address: CRTBT, 25 avenue de Martyrs, BP 166X, 38084 Grenoble Cedex, France.

¶ Permanent address: Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau Cedex, France.

0305-4470/89/132577+09$02.50

these limits the standard parametrisation (βJ, Δ) may be misleading while this is not the case for the homogeneous one (see below).

For the square lattice, in the thermodynamic limit, the model has some obvious symmetries which correspond to the following permutations of the $w(i)$:

$$T: w(0) \to w(1) \to w(2) \to w(0) \tag{2a}$$

and

$$S: w(1) \leftrightarrow w(2). \tag{2b}$$

A duality transformation can be defined for this model by (Wu and Wang 1976)

$$D: \hat{w}(n) = \sum_{p=0}^{2} \omega^{np} w(p) \tag{3}$$

where ω is a cube root of unity, $\omega^3 = 1$. D is a transformation of order four. As a particular case of Au Yang *et al* (1987) and Baxter *et al* (1988), the model satisfies a star-triangle relation provided a homogeneous algebraic relation between the $w(i)$ is satisfied:

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

As a consequence of a more general conjecture of Baxter *et al* (1988) and confirmed by Baxter (1988) about the critical variety of the integrable anisotropic N-state chiral Potts model, there is only one critical point when one restricts the parameter space to the algebraic variety defined by (4). This point is nothing but the critical ferromagnetic point of the standard scalar Potts model (Baxter 1982*a*) (point H in figure 1(*a*)) which actually lies on (4). Other sets of points are relevant to the study of the isotropic model presented here:

(*a*) the line where the model reduces to the scalar Potts model $w(1) = w(2)$

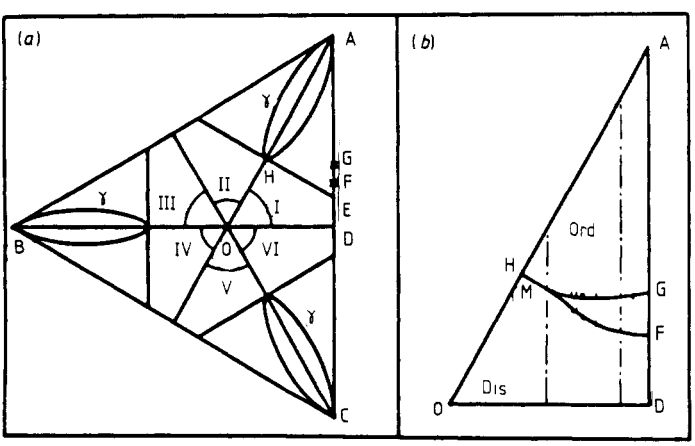

Figure 1 (*a*) Phase diagram of the three-state chiral Potts model in the (a, b) plane where a and b are defined by (6). The inside of the triangle corresponds to the physical domain. On line AO the chiral model reduces to the standard scalar Potts model. Line HE is the self-dual line (5). Curve γ corresponds to the star triangle condition (4). (*b*) Sector I 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 chain lines correspond to the sweeps for $a = 0.20$ and $a = 0.35$.

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

$$\sqrt{3}w(0) = w(0) + w(1) + w(2) \tag{5}$$

and its transforms by T and T^2.

The $w(i)$ are homogeneous variables, so it is convenient because of the symmetries ($2a$, b), to parametrise the model in the two reduced variables defined by

$$\begin{aligned} a &= (w(0) - 2w(1) + w(2))/\sqrt{6}(w(0) + w(1) + w(2)) \\ b &= (w(0) - w(2))/\sqrt{2}(w(0) + w(1) + w(2)). \end{aligned} \tag{6}$$

In the (a, b) plane the physical domain is restricted to the triangle drawn on figure 1(a), where we have also drawn the standard scalar Potts line, the self-dual line (5), their transformations by T and T^2 and curve (4). Because of the symmetries ($2a$, b) one restricts the study of the phase diagram to the triangle AOD (sector I). The edges (AO), (OD), (DA) of this triangle correspond, respectively, to the isotropic three-state ferromagnetic standard scalar Potts model ($w(0) > w(1) = w(2)$), to the isotropic three-state antiferromagnetic standard scalar Potts model ($w(1) < w(0) = w(2)$) and to a limit where the chiral model can be mapped in the thermodynamic limit onto a six-vertex model in direct fields. Point A ($w(1) = w(2) = 0$) corresponds to a completely ordered state while point O corresponds to the completely disordered one. Point D is the completely ordered limit of the antiferromagnetic scalar Potts model.

Kardar (1982) has considered an N-state isotropic helical Potts model with Hamiltonian:

$$-\beta H = \sum_{\langle ij \rangle} J\delta(\sigma_i - \sigma_j) + W\delta(\sigma_i - \sigma_j + 1) \tag{7}$$

where σ_i belongs to $\mathbb{Z}_N$ and δ denotes the Kronecker symbol. For $N = 3$ this is another way to define the chiral Potts model. Kardar made the remark that, when oriented neighbouring spin pairs are either in the same state (i, i) or with spins differing by 1 (i, $i+1$), this N-state helical Potts model can be mapped onto a six-vertex model in direct equal horizontal and vertical fields (figure 1 of Kardar (1982)). He got this situation by taking the limit $J \to \infty$, $W \to \infty$. This limit of the model corresponds (in sector I) to the *two* points, D: $a = 1/\sqrt{6}$, $b = 0$ ($w(0) = w(2)$, $w(1) = 0$) and A: $a = 1/\sqrt{6}$, $b = 1/\sqrt{2}(w(1) = w(2) = 0)$. We note that this mapping may be extended (even for the N-state chiral Potts model) to the whole boundary $a = 1/\sqrt{6}$ (i.e. $w(1) = 0$). This mapping onto the six-vertex model can be made rigorous (especially for finite-size systems) by taking care of the boundary conditions. Recalling the analysis of the six-vertex model in a direct field performed by Sutherland *et al* (1967) and Yang (1967), one locates a critical point on this $w(1) = 0$ limit (ice point) for $w(0)/2w(2) = 1$. This corresponds to $b = 1/3\sqrt{2} = 0.235$. Note that this point (G in figure 1(a, b)) is rather far from the self-dual line (5) (point E). Another known result concerns point D which corresponds to the critical antiferromagnetic scalar Potts model for $N = 3$: $(e^J + 1)^2 = 4 - N$ (Baxter 1982b). At this point the order-disorder transition is of infinite order (Kosterlitz-Thouless type) (den Nijs *et al* 1982). No other point is expected to be critical on the OD boundary.

Often, for isotropic models in two dimensions, criticality, integrability and self-duality are notions having some overlap. Examples are the scalar Potts model, Ashkin-Teller models or $\mathbb{Z}_n$ models (Baxter 1982a, Zamolodchikov and Monarstirskii 1979, Zamolodchikov and Fateev 1985). So the first question addressed below concerns the criticality of the model on condition (4).

Using (14) of Kardar (1982) one can argue that there should *exist* at least a phase boundary close to point H given in the neighbourhood of H by

$$J - W/2 = \ln(1+\sqrt{3}). \tag{8}$$

Written in the homogeneous variables $w(i)$, (8) simply means that the critical curve is orthogonal to the line AO. Indeed, this is related to the $w(1) \leftrightarrow w(2)$ symmetry (if point H is regular). Note that such a critical curve is therefore tangent to the self-dual line (5). Hence a question is of interest: is there a critical curve connecting the two critical points H and G?

To investigate these questions we have performed Monte Carlo simulations on a parallel computer build in the Centre de Recherche sur les très basses tempèratures, Grenoble (CRTBT). This computer allows us to average the results over a rather large number of samples. We now describe the method used. We study $L \times L$ square lattices with helical boundary conditions. As already noticed above, in the equilibrium configuration at point A all the spins are of the same colour. So one can expect that, starting a Monte Carlo run not too far from A with all the spins of the lattice of the same colour, the equilibrium will be reached after a short time (note that it is no longer the case on the $w(1) = 0$ boundary where the local Monte Carlo algorithm cannot work). One can check that the system has reached the equilibrium making use of the fluctuation-dissipation theorem. For most of the simulations presented here we start from a point (a_0, b_0) which lies not too far from A. Then to sample the equilibrium for a point (a, b) near (a_0, b_0) we use a standard Metropolis method (Metropolis *et al* 1953): a spin σ_i is randomly chosen, and its colour is updated to a new colour k with probability

$$P(\sigma_i = k) = w(\sigma_{i+L} - k)w(\sigma_{i+1} - k)w(k - \sigma_{i-1})w(k - \sigma_{i-L})/z \tag{9}$$

where z ensures the normalisation of P.

Because of the length of the simulations performed here ($>10^{11}$ updates in some runs) the random number generation can become important (Barber *et al* 1985). The random number generator we use here is the XOR generator (Pearson *et al* 1983) with parameters 607 and 297. Moreover, the architecture of our computer allows us to perform completely independent runs, each of them using its own random number sequence.

With the helical boundary conditions the spins are indexed such that σ_{i+L}, σ_{i+1}, σ_{i-1}, σ_{i-L} are the four nearest neighbours of σ_i. The first steps are discarded, as a transient regime to the equilibrium. Then we compute the 'internal energy' e of a configuration of spins defined as

$$e = -\sum P_\nu \ln[w(\nu)/(w(0)+w(1)+w(2))] \tag{10}$$

where the sum is performed over all oriented bonds and $P_\nu = N_\nu/2L^2$, N_ν being the number of bonds for which the oriented neighbouring spin pairs correspond to $(\sigma_i, \sigma_i + \nu)$ and L denotes the linear size of the square sample. The fluctuations of this quantity are similar to a 'specific heat', and this allows us to obtain a criterion to localise the critical points. We also compute a magnetisation and its fluctuation.

The lattices considered here have different sizes $L \times L$: $L = 4, 8, 16, 32, 64$. Typically the sweeps in the (a, b) plane considered in this paper correspond to keeping constant the value of a and to decrement b by steps of 2.5×10^{-3}. A measure of $\langle e \rangle$ and $\langle e^2 \rangle$ is performed for all ten Monte Carlo steps (MCS) per spins. For instance, in the case $L = 64$ (16) 5000 MCS per spins are discarded to (to thermalise the system) and 10^8 (4×10^8) values are averaged. For the $L = 64$ case, for instance, it represents 4×10^{11}

updates and it took three weeks (for a given value of a) on the parallel computer of the CRTBT, which consists of 46 M68000 working in parallel (the total number of updates corresponding to all the simulations performed in this work is 5×10^{12}). The program written in assembly language needs about 50 instructions, representing 400 clock periods, for a single update.

To check the validity of our program and also the relevance of the internal energy (10) and of the temperature-like variable b we have performed different runs (for $L=8$, 16, 32) along trajectories in the parameter space corresponding to the standard scalar Potts model ($b=\sqrt{3}\,a$, AO in figure 1(a)) as well as a sweep for a given value of a ($a=a_H=(\sqrt{3}-1)/6\sqrt{2}$), some with our variables and others with conventional variables. The finite-size scaling analysis in the two cases leads to the same conclusions, namely that the determination of the critical point is good, but that the exponents are more difficult to extract. More precisely, despite the fact that we discard the few points out of equilibrium (using the criterion previously mentioned) we have found $b_c\sim0.150$, $1/\nu\sim1.0$ and $\alpha/\nu\sim0.5$, while the exact values are $b_c=0.149$, $1/\nu=1.2$ and $\alpha/\nu=0.4$. These discrepancies in the value of exponents are due to important corrections to scaling, as already mentioned by Barber (1988).

To investigate the criticality of the integrability curve (4) we have performed sweeps for $a=0.20$ and different values of L ($L=4$, 8, 16, 32, 64). The same calculations have also been performed for $a=0.25$ with similar results. The results are shown in the insert of figure 3: $c(b)$ presents a maximum which becomes sharper with increasing values of L. We found that the susceptibility also exhibits a sharp maximum. The system seems to undergo a second-order phase transition between an ordered and a disordered phase. The size effects are characteristic of such a transition and this is confirmed by a representative spin configuration just above the transition (see figure 2(a)). Moreover, the value of b corresponding to the integrability curve $b_{\rm int}(a=0.20)=0.275$ is clearly to be discarded as well as the self-dual value $b_{\rm sd}(a=0.20)=0.2296$, while the maxima of the specific heat are found to range from $b(L=4)=0.2250$ to $b(L=64)=0.2375$. This shows that the simplicity argument, which would have identified the critical curve with the self-dual line, fails. This also shows that curve (4), if critical for the chiral three-state Potts model, corresponds to a very weak singularity. One could think of a connection between this curve and a wetting transition curve (compare, up to the change of variables, curve (4) in figure 1 and figure 1 of Huse *et al* (1983)). On the other hand, these results suggest that the critical curve is located close to the self-dual line near $a=0.20$. A finite-size scaling analysis of our results (see figure 3) leads to the following values: $b_c(a=0.20)\sim0.240$, $1/\nu\sim1$ and $\alpha/\nu\sim0.5$. As in the standard scalar Potts model these exponents are not very reliable (in particular they violate the hyperscaling relation $d\nu=2-\alpha$). The close similarity of these results with the one obtained along the OA boundary (standard scalar Potts model) does not allow one to rule out a transition (at least near this value of a) in the same universality class as the standard scalar Potts model.

In order to follow this transition for larger values of a, Monte Carlo simulations were carried out for $L=16$ and $a=0.35$. The situation now seems more involved. Indeed, as shown in figure 4, $c(b)$ exhibits two maxima. The first one occurs for $b_1=0.1474$ while the second one occurs for $b_2=0.214$. These numbers are to be compared with $b_{\rm sd}(a=0.35)=0.143$. b_2 is rather far from $b_{\rm sd}$ and indicates a critical phase boundary going up to point G. For $L=32$ we get then three maxima with increasing amplitudes with b. For $L=64$ we get six maxima, also with increasing amplitudes as b increases. These striking results indicate a rather involved phase

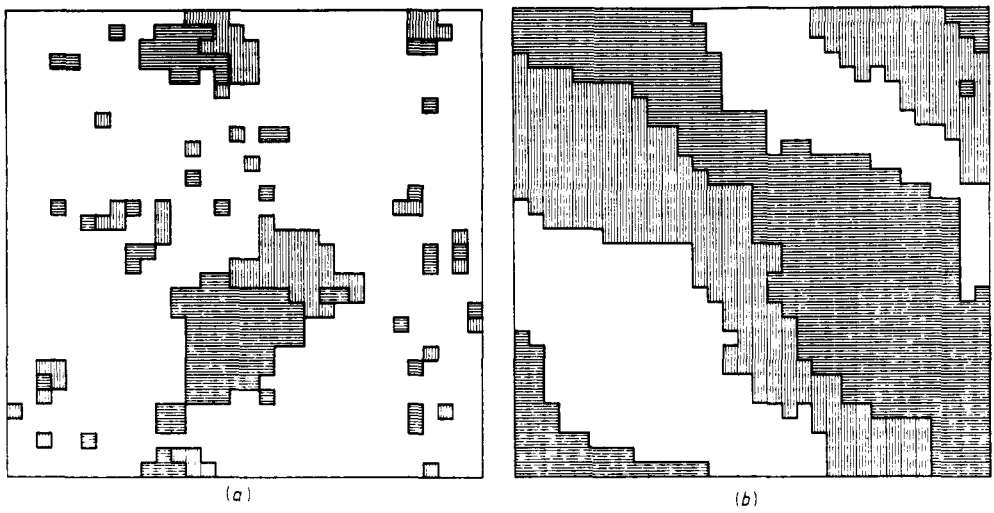

Figure 2. (*a*) Snapshot for $a = 0.20$ and $b = 0.230$. (*b*) Snapshot for $a = 0.35$ and $b = 0.200$. (*c*) Snapshot for $a = 0.35$ and $b = 0.185$.

structure for $a = 0.35$ in a certain range $\{b_{\min}, b_{\max}\}$ in b. A difference between the order breaking mechanism of the system (as b is decreased) also appears while comparing the snapshots of the spin configurations of the system for $a < 0.2$ and for $a > 0.2$. For example, typical snapshots are given in figure 2(a, b, c) for $a = 0.20$ and $a = 0.35$. For $a = 0.20$ this breaking takes place through flips of isolated clusters of spins. For sectors I and II the ordered phase (greatest values of b) corresponds to a ferromagnetic state, while for sector III and IV (V and VI) it corresponds to an helical state (Kardar 1982) $\langle \ldots 012 \ldots \rangle$ ($\langle \ldots 021 \ldots \rangle$). For $a = 0.35$ a very large number of spins organised in walls running diagonally through the lattice are involved. This is reminiscent of a floating phase. With our choice of boundary conditions the number of walls must be divisible by three. The values of b corresponding to a maximum of

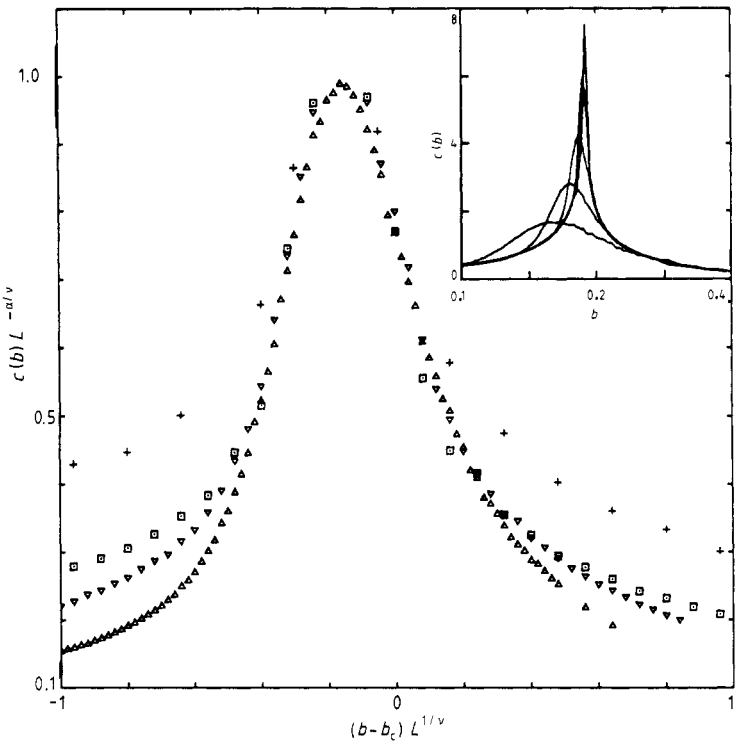

Figure 3. Finite-size scaling for $c(b)$ for $a = 0.20$ and $L = 8(\triangle)$, $16(\triangledown)$, $32(\boxdot)$, $64(+)$ with $1/\nu = 1$ and $\alpha/\nu = 0.5$. The insert shows the original data.

$c(b)$ are precisely the ones for which the number of walls increases by three. Moreover, in this phase the setting of the equilibrium seems to be slower. It has been verified for trajectories in the parameter space allowing an easy use of the fluctuation-dissipation theorem which corresponds to a given chirality $\Delta = -0.42$ (Anglès d'Auriac *et al* 1989). Note that the run performed for $L = 16$ already gave a reliable estimation of the extension of this 'new phase'. With the aim to precisely determine the extension of this 'new phase' in the phase diagram, sweeps for $a = 0.26$, 0.265, 0.270, 0.275, 0.30, 0.37, have been carried out for $L = 16$. All these simulations indicate two maxima which must trace the location of $\{b_{\min}, b_{\max}\}$. As shown in figure 1(b), they confirm that, at least for $a > 0.25$, such a phase could occur.

Let us now discuss the results presented in this paper. From exact results we have located certain critical points of the isotropic three-state chiral Potts model. We have shown, using a Monte Carlo simulation, that these points are, in fact, connected by continuous phase boundaries which define, in the phase diagram, ordered phases and a domain where the phase structure is involved and reminiscent of a floating phase. We have verified that increasing the size of the lattice from $L = 16$ up to $L = 64$, this phase structure persists. This seems to exclude a metastability leading to spurious behaviour for the specific heat. Two possibilities are consistent with the evidence we have obtained.

(a) The floating phase begins at a value $a = a_M \sim 0.2$ (see figure 1(b)). For $a < a_M$ there is a only one order-disorder transition which could be in the standard scalar Potts universality class.

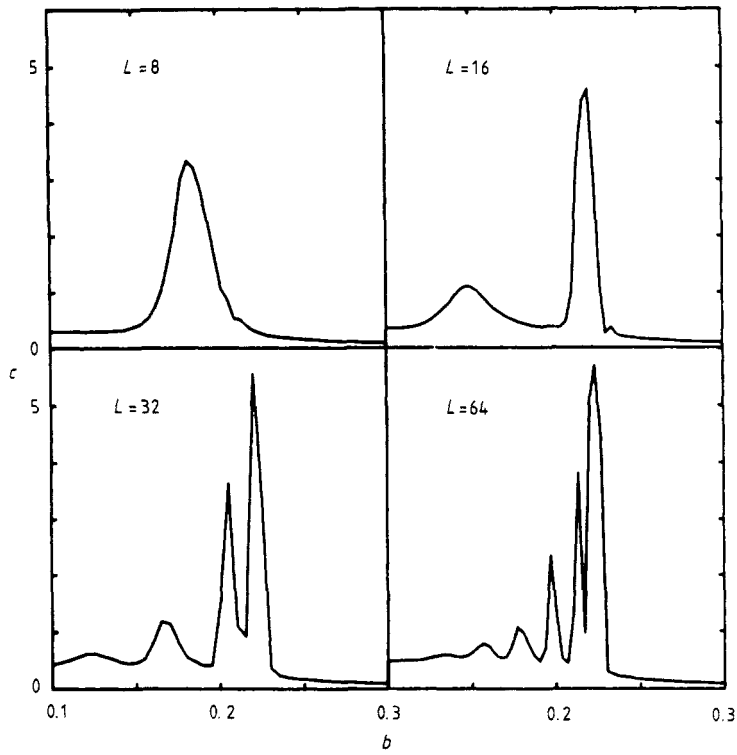

Figure 4. $c(b)$ for different values of L.

(b) The critical ferromagnetic standard scalar Potts point H is, in fact, a multicritical point. In this case the two critical curves originated at point H are hardly distinguishable up to a_M (of course, such a situation should lead to some anomalies in the finite-size scaling analysis).

The last situation seems to be the most likely. On the other hand, a certain ambiguity remains on the precise localisation of point F. This ambiguity is difficult to clarify since the local Monte Carlo algorithm fails in the neighbourhood of the AD line. It is not proved that point F is definitely different from point E or even D.

One must remember that the very existence of modulated or floating phases in two-dimensional isotropic models is still a matter of controversy (Oitmaa and Velgakis 1988, Velgakis and Oitmaa 1988). Hence other studies are necessary to have a better understanding of this intermediate phase. A simulation for a 128×128 lattice is in progress (Anglès d'Auriac *et al* 1989).

To conclude, the finite-size scaling analysis has shown that the self-dual line is not critical. The criticality of self-dual lines was natural for $\mathbb{Z}_n$ models (Zamolodchikov and Monastirskii 1979, Zamolodchikov and Fateev 1985) because these lines are not only globally invariant by duality but each of their points are invariant: this is no longer the case for chiral models. However, let us emphasise that the algebraic nature of critical boundaries 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). Critical curve(s) have been located with accuracy for $a < 0.2$. The analysis performed to get the exponents ν and α does not allow us to rule out at the present moment the fact that the isotropic three-state chiral Potts

model could be, near point H, in the same universality class as the standard scalar Potts model. On the other hand, the precise extension of the 'floating phase' is more difficult to estimate.

Finally let us note that it would be of some interest to study other chiral Potts models for $N > 3$. Especially for $N = 4$ one can see that the phase diagram is very involved by inspecting different limits which correspond to exactly known results (Ashkin-Teller limit, six-vertex model in direct fields).

Acknowledgments

We would like to thank Professor R Rammal for many discussions, Dr P Rujan for useful comments and mentioning the paper by M Kardar and R Bourbonnais for a critical reading of the manuscript.

References

Anglès d'Auriac J C, Hansel D and Maillard J M 1989 in preparation
Au-Yang H, McCoy B M, Perk J H H, Tang S and Yan M L 1987 *Phys. Lett.* **123A** 219
Barber M N 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowitz (New York: Academic) p 145
Barber M N, Pearson R B, Toussaint D and Richardson J L 1985 *Phys. Rev.* B **32** 1720
Baxter R J 1982a *Exactly Solvable Models in Statistical Mechanics* (New York: Academic)
—— 1982b *Proc. R. Soc.* A **383** 43
Baxter R J 1988 *J. Stat. Phys.* **52** 639-67
Baxter R J, Perk J H H and Au Yang H 1988 *Phys. Lett.* **128A** 138
Everts H U and Röder H 1989 A quantum version of the chiral clock model: the paramagnetic to commensurate transition *Z. Phys.* submitted
von Gehlen G and Rittenberg V 1985 *Nucl. Phys.* B **257** 351
Hoeger C, von Gehlen G and Rittenberg V 1985 *J. Phys. A: Math. Gen.* **18** 1813
Huse D A 1981 *Phys. Rev.* B **24** 5180
Huse D A, Szpilka A M and Fisher M E 1983 *Physica* **121A** 363
Kardar M 1982 *Phys. Rev.* B **26** 2693
Metropolis N, Rosenbluth A W, Rosenbluth M N, Teller A H and Teller E 1953 *J. Chem. Phys.* **21** 1087
den Nijs M 1988 *Phase Transition and Critical Phenomena* vol 12, ed C Domb and J L Lebowitz (New York: Academic) p 219
den Nijs M, Nightingale M P and Schick M 1982 *Phys. Rev.* B **26** 2490
McCoy B M, Perk J H H, Tang S and Sah C H 1987 *Phys. Lett.* **125A** 9
Oitmaa J and Velgakis M J 1987 *J. Phys. A: Math. Gen.* **20** 1495
Ostlund S 1981 *Phys. Rev.* B **24** 398
Pearson R B, Richardson J L and Toussaint D J 1983 *J. Comput. Phys.* **51** 241
Selke W 1988 *Phys. Rep.* **170** 213
Selke W and Yeomans J M 1982 *Z. Phys.* B **46** 311
Sutherland B, Yang C N and Yang C P 1967 *Phys. Rev. Lett.* **19** 588
Velgakis M J and Oitmaa J 1988 *J. Phys. A: Math. Gen.* **21** 547
Wu F Y and Wang Y K 1976 *J. Math. Phys.* **17** 439
Yang C P 1967 *Phys. Rev. Lett.* **19** 586
Zamolodchikov A B and Fateev V A 1985 *Sov. Phys.-JETP* **62** 215
Zamolodchikov A B and Monarstirskii M I 1979 *Sov. Phys.-JETP* **50** 167