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Critical behaviour of a (1 + 1) dimensional Potts model with ferromagnetic and antiferromagnetic interactions

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Abstract. We study the one-dimensional quantum Hamiltonian version of a two-dimensional three-state Potts model on a square lattice which has ferromagnetic interactions in the x direction and antiferromagnetic interactions in the y direction in the limit of strong coupling in the x direction. We find a massless low-temperature behaviour. The transition point which has an essential singularity is located at a different point as previously conjectured.

1. Introduction

The purely antiferromagnetic two-dimensional q -state Potts model (Wu 1982) has been of great interest in the past because of its rich features: a ground state with a complicated degeneracy and an essential singularity for $q = 3$ (Nightingale and Schick 1982) and on the other hand, an exactly known transition line for $q \leq 3$ (Baxter 1982).

A mixed Potts model on a square lattice in which only the couplings in the y direction are antiferromagnetic while the couplings in the x direction are ferromagnetic has been less studied, although it might be equally rich as the purely antiferromagnetic model and less difficult to handle numerically. The transition line is not exactly known but a conjecture was made by Kinzel *et al* (1981):

$$(1 + e^{J_x})(1 - e^{J_y}) = q, \quad (1)$$

where $J_x > 0$, $J_y < 0$ are the dimensionless coupling constants. On the other hand, contrary to the purely antiferromagnetic case, the degeneracy of the ground state can easily be calculated. Numerically a Migdal-Kadanoff renormalisation group and a Monte Carlo simulation for $q = 3$ have been performed on the mixed Potts model (Kinzel *et al* 1981), the first supporting the conjecture (1) and the second suggesting an unconventional transition.

In order to clarify the situation of the mixed Potts model, we will investigate in this paper the case $q = 3$ by solving the one-dimensional quantum Hamiltonian version of the model, i.e. in the limit $J_y \rightarrow 0$, $J_x \rightarrow \infty$ with $J_y e^{J_x}$ fixed and extrapolating the results with finite size scaling arguments (Hamer and Barber 1980, Herrmann 1981).

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This method is related to the phenomenological renormalisation (Nightingale 1982, Sneddon and Stinchcombe 1979) and has been successful because of its numerical accuracy. Furthermore the quantum Hamiltonian is in itself interesting as a model.

In § 2 we describe the model and explain the method, § 3 is devoted to the results and § 4 summarises and concludes.

2. Model and method

We begin by considering the classical two-dimensional anisotropic q -state Potts model on a square lattice:

$$-\beta H = \sum_{\langle i,j \rangle} (J_y \delta_{\sigma_i, \sigma_j} + J_x \delta_{\sigma_i, \sigma_j}), \quad \sigma_i = 1, \dots, q, \quad (2)$$

with general, i.e. ferromagnetic or antiferromagnetic, couplings J_x and J_y . To go over to the one-dimensional quantum version of (2) we choose the x direction as 'time' direction (Fradkin and Susskind 1978, Sneddon and Stinchcombe 1979) and have to describe the transfer operator in the x direction in the form of an exponential

$$T_x = \prod_i \left(\mathbf{1}_i e^{J_x} + \sum_{l=1}^{q-1} t_i^l \right) \propto \exp[(K_x/q)A] \quad (3)$$

where

$$t_i = \begin{pmatrix} 0 & 1 & \dots & 0 \\ & & \dots & 1 \\ 0 & & \dots & 0 \\ 1 & 0 & \dots & 0 \end{pmatrix}_i$$

and $\mathbf{1}$ is the unity operator. One quickly sees by looking at the eigenvalues of T_x that this is only possible if $J_x > 0$. So we have to choose our time direction to have the ferromagnetic coupling. This also explains why the purely antiferromagnetic Potts model cannot be studied in a quantum version. From (3) one gets

$$A = \sum_i \sum_{l=1}^{q-1} t_i^l \quad (4)$$

and

$$e^{K_x} = [1 + (q-1)e^{-J_x}]/(1 - e^{-J_x}). \quad (5)$$

The complete transfer matrix T is composed of T_x and the contribution of the couplings within the y direction:

$$T \propto \exp(J_y B) \exp[(K_x/q)A], \quad B = \sum_i \delta_{\sigma_i, \sigma_{i-1}}. \quad (6)$$

Thus no condition is imposed on the J_y and we choose it to be the antiferromagnetic coupling of the mixed Potts model.

The quantum Hamiltonian \mathcal{H} is obtained by writing T as an exponential

$$T \propto \exp[-(J_y/q)\mathcal{H}] \quad (7)$$

which is done by use of the Baker–Hausdorff formula

$$\exp(J_y B) \exp[-(\lambda/q)J_y A] = \exp\{J_y[B - (\lambda/q)A]\} \exp[(\lambda/2q)J_y^2[B, A] + O(J_y^3)] \quad (8)$$

in the limit of $J_y \rightarrow 0$ with $\lambda = -K_x/J_y$ fixed. The second factor of the right-hand side of (8) contains many operators composed of commutators which because of their higher powers in J_y can usually be neglected unless they are not irrelevant, i.e. if they destroy the degeneracy of the ground state. This is if one deals with a highly degenerate ground state a delicate question. In our case one can see that none of the commutators appearing in (8) is relevant and thus the procedure is correct. But the easiest way to convince oneself of the equivalence of the one-dimensional quantum Hamiltonian

$$\mathcal{H} = \lambda A - qB \quad (9)$$

that one gets from (7) and the two-dimensional classical model (2) is counting for both cases the degeneracy of the ground state. For a strip of width N in (2) and for a chain of N sites in (9) the degeneracy is in both cases $q(q-1)^{N-1}$. The quantum Hamiltonian (9) differs from the quantum Hamiltonian of the common ferromagnetic Potts model (Herrmann 1981) only by a relative sign between the operators A and B .

It is numerically more convenient to work in another basis (Sólyom and Pfeuty 1981), and then the Hamiltonian becomes modulo a constant

$$\hat{\mathcal{H}} = \sum_i \sum_{k=1}^{q-1} t_i^k t_{i+1}^{q-k} - \lambda \sum_i u_i \quad (10)$$

with

$$u_i = \begin{pmatrix} q-1 & & & 0 \\ & -1 & & \\ & & \ddots & \\ 0 & & & -1 \end{pmatrix}$$

In the limit $J_y \rightarrow 0$ with fixed λ equation (5) goes over to

$$K_x = q e^{-J_x}$$

and thus the conjecture (1) of Kinzel *et al* (1981) for the critical point becomes

$$\lambda_c = 1 \quad (11)$$

for the quantum models (9) or (10).

It is known (Fradkin and Susskind 1978, Kogut 1979) that the ground state energy density and the energy gap of the one-dimensional quantum model are proportional to the free energy density and the reciprocal correlation length of the two-dimensional classical model respectively. So it suffices to calculate the two lowest-lying energy levels E_0 and E_1 of the quantum Hamiltonian (10) to get all the interesting information on the classical model (2). Our approach consists in calculating E_0 and E_1 exactly on a chain of N sites. We use open chains because periodic boundary conditions would change the ground state degeneracy and introduce a strong even-odd parity. Unfortunately finite size effects are stronger in the case of open chains (Fisher 1971).

The numerical task thus consists in obtaining the two largest eigenvalues of $q^N \times q^N$ matrices. This is done by an iterative algorithm; for technical details see Herrmann (1981). We only treat the case $q = 3$ and go up to $N = 8$.

3. Results

The gap for a chain of N sites

$$G_N = E_0 - E_1 \tag{12}$$

is shown against λ in figure 1. If (11) defines the critical point as conjectured (Kinzel *et al* 1981) this gap should go to zero at $\lambda = 1$. Figure 1, however, suggests that the gap vanishes at much smaller values of λ .

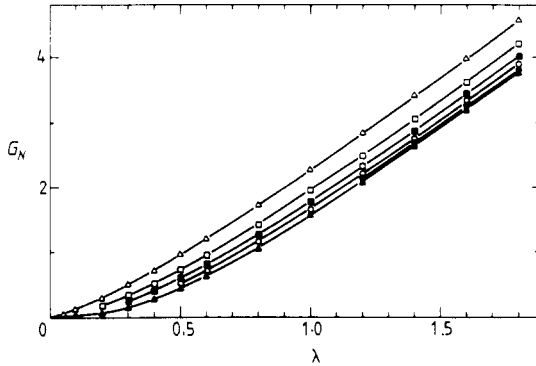


Figure 1. Gap plotted against coupling parameter λ for different chain lengths N . Δ , $N = 2$; \square , $N = 3$; \blacksquare , $N = 4$; \circ , $N = 5$; \bullet , $N = 6$; \blacktriangle , $N = 7$.

Next we will analyse the gap using finite size scaling arguments (Jullien and Pfeuty 1981):

$$G_N \sim N^{-z} f(N^{1/\nu}(\lambda - \lambda_c)). \tag{13}$$

f is a scaling function and ν the exponent of the correlation length of the classical model. The ‘dynamical’ exponent z is the ratio of ν_t —the exponent of the correlation length in the ‘time’ direction—and ν . As our Hamiltonian is equivalent to a classical model, z must be one because G^{-1} is proportional to the correlation length. Also figure 2, where G_N is double-logarithmically plotted against N , shows that the straight lines have slope $z = 1$ (compare with the guides to the eye (broken lines) of slope one). From (13) one expects in figure 2 a straight line only at the critical point. This excludes a λ_c larger than 0.3, in support of our conclusions from figure 1. But for λ_c smaller than 0.3 all the curves can be asymptotically straight for large N which indicates a line of critical points. Looking at NG_N against λ in figure 3 (Roomany and Wyld 1980) one also does not find one fixed point for different chain lengths but a whole line of pseudo-fixed points for small λ and a trivial fixed point at $\lambda = 0$. Figures 2 and 3 thus exclude the existence of one single isolated critical point at a finite λ and suggest a special region at small λ .

Next we examine the critical behaviour in the region of small λ . The exponent ν of the classical correlation length is calculated from (13) by

$$G_N (\partial G_N / \partial \lambda)^{-1} \sim N^{-1/\nu}. \tag{14}$$

Note that (14) does not depend on z .

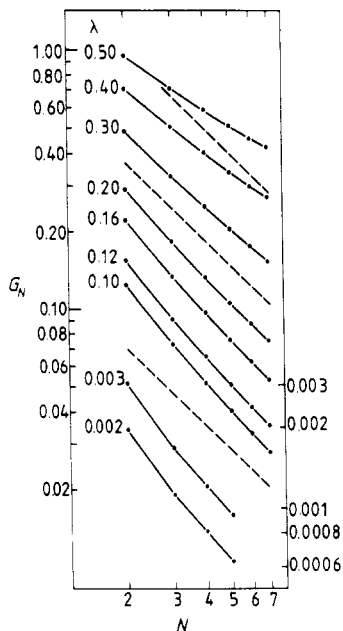


Figure 2. Double-logarithmical plot of the gap G_N against chain length N for different values of λ . The left scale of the G_N axis is for $\lambda \geq 0.1$, the right scale for $\lambda \leq 0.003$.

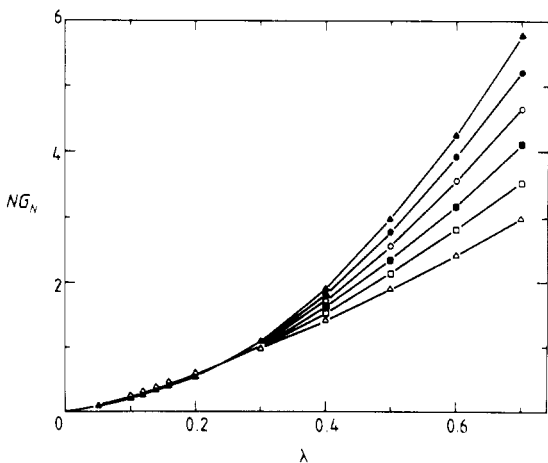


Figure 3. NG_N plotted against λ for different chain lengths N . Δ , $N=2$; \square , $N=3$; \blacksquare , $N=4$; \circ , $N=5$; \bullet , $N=6$; \blacktriangle , $N=7$.

In figure 4 we show the double-logarithmical plot of $G_N (\partial G_N / \partial \lambda)^{-1}$ against N for different values of λ . The slope of the curves for $\lambda < 0.05$ clearly yields an infinite ν but also for $\lambda < 0.2$ one might get $\nu \rightarrow \infty$ for large N . We conclude that for small λ we have a diverging correlation length, i.e. a line of critical points. This suggests a massless phase with an essential singularity at a $\lambda_c < 0.2$ (Jullien and Pfeuty 1981).

Figure 5 shows the ‘specific heat’

$$C = -d^2 \epsilon_0 / d\lambda^2 \tag{15}$$

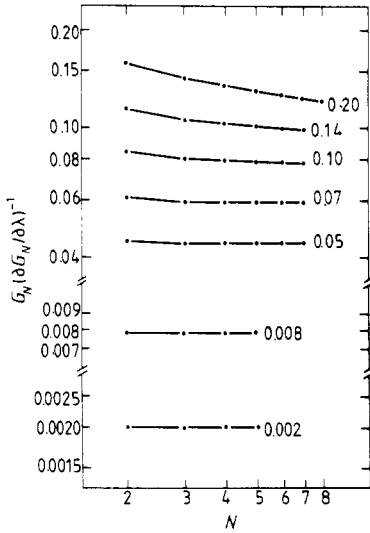


Figure 4. Double-logarithmical plot of $G_N (\partial G_N / \partial \lambda)^{-1}$ against N for different values of λ .

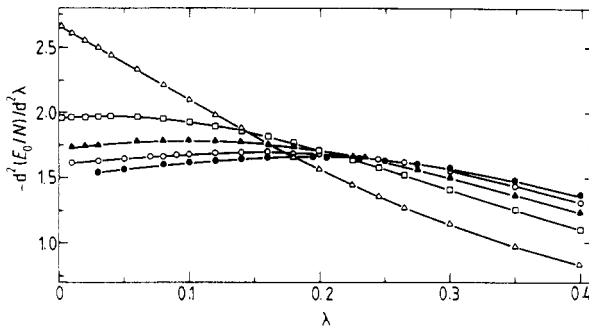


Figure 5. Specific heat plotted against λ for different chain lengths N . Δ , $N = 2$; \square , $N = 3$; \blacktriangle , $N = 4$; \circ , $N = 5$; \bullet , $N = 6$.

where $\varepsilon_0 = E_0/N$ is the ground state energy density. Clearly the specific heat does not diverge in the critical region of small λ . This is also typical for a massless phase.

In summary we conclude from figures 4 and 5 that there is a region of small λ showing massless behaviour and that the transition at λ_c to this region has an essential singularity. We thus agree with the statement made by Kinzel *et al* (1981) that the transition is of ‘unconventional type’. It is, however, difficult to determine the extent of the massless region.

A more precise determination of the transition point is possible by looking at the function

$$\beta(\lambda) \equiv d\lambda/da \tag{16}$$

(Nightingale and Schick 1982), where a is the rescaling factor between two chains of different length, explicitly:

$$da = -dN/N. \tag{17}$$

Using the usual renormalisation equation for chains of sizes N and N' (see e.g. Derrida and de Seze 1982) and (13) (with $z = 1$) yields

$$NG(\lambda) = N'G_{N'}(\lambda'). \tag{18}$$

From (16)–(18) one obtains

$$\beta(\lambda) = \frac{1 + \partial \ln G_N / \partial \ln N}{\partial \ln G_N / \partial \lambda} \tag{19}$$

and the numerical approximation of the derivatives for a pair of chains of N and $N + 1$ sites yields

$$\beta_{N,N+1}(\lambda) = \frac{1 + \ln(G_N/G_{N+1})/\ln(N/N+1)}{[(\partial G_N/\partial \lambda)(\partial G_{N+1}/\partial \lambda)/G_N G_{N+1}]^{1/2}} \tag{20}$$

The function β vanishes at the fixed point of (18). In figure 6 we show the functions $\beta_{N,N+1}$ for different pairs N and $N + 1$. The conclusions we drew from figures 4 and 5 about the critical behaviour of the model imply that in the limit $N \rightarrow \infty$ the curves $\beta_{N,N+1}$ will tend to a function which is zero for $\lambda < \lambda_c$. Figure 6 shows that such an asymptotic behaviour is quite plausible. The points $\lambda_c(N, N + 1)$ at which $\beta_{N,N+1}$ crosses the zero axis will then tend towards λ_c . In the inset we plotted $\lambda_c(N, N + 1)$ against N^{-1} . There is clearly a slight even–odd imparity in the $\lambda_c(N, N + 1)$. To get rid of this we also calculated $\lambda_c(N, N + 2)$ and plotted it in the inset of figure 6. $\lambda_c(N, N + 1)$

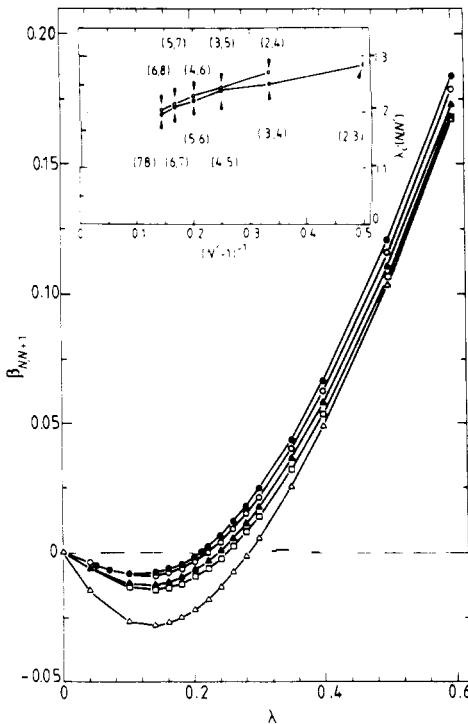


Figure 6. Function $\beta_{N,N+1}$ plotted against λ for different pairs $N, N + 1$. ($N, N + 1 = 2, 3$ (Δ); 3, 4 (\square); 4, 5 (\blacktriangle); 5, 6 (\circ); 6, 7 (\bullet)). The inset shows $\lambda_c(N, N')$ plotted against $(N' - 1)^{-1}$ for $N' = N + 1$ (full circles) and $N' = N + 2$ (open circles).

and $\lambda_c(N, N + 2)$ can both be extrapolated to $N \rightarrow \infty$ and yield $\lambda_c < 0.13$. It is, however, not possible to exclude from this extrapolation $\lambda_c = 0$. The difficulties in the extrapolation arise from the fact that the finite size effects are very strong due to the free ends of the finite chains.

In the infinite system we have at λ_c the essential singularity

$$G \sim \exp[-a(\lambda - \lambda_c)^{-\sigma}] \tag{21}$$

and so the function β behaves as

$$\beta(\lambda) \sim (\sigma a)^{-1}(\lambda - \lambda_c)^{\sigma+1}. \tag{22}$$

In figure 7 we plot $\beta_{N,N+1}$ double logarithmically against $\lambda - \lambda_c^*$ for different tentative values of λ_c^* . For large N , equation (22) predicts a straight line of slope $\sigma + 1$ at $\lambda_c^* = \lambda_c$. Unfortunately for the values of N that we consider the curves do still change considerably with N as shown in figure 7. For $N = 7$ and $\lambda_c^* = 0.2$ one has nearly a straight line but for larger N the curve for $\lambda_c^* = 0.2$ will not be straight any more. It is not easy to say for which λ_c^* the curve will become a straight line in the limit $N \rightarrow \infty$. But clearly an upper limit for λ_c is 0.2 in agreement with our previous findings. Because of the uncertainty in λ_c and the strong finite size effects the exponent σ cannot be reliably extracted. To estimate an upper limit for σ we look at the slope of the curve for $\lambda_c^* = 0$ in the region where finite size effects are strong. This gives us $\sigma < 0.9$.

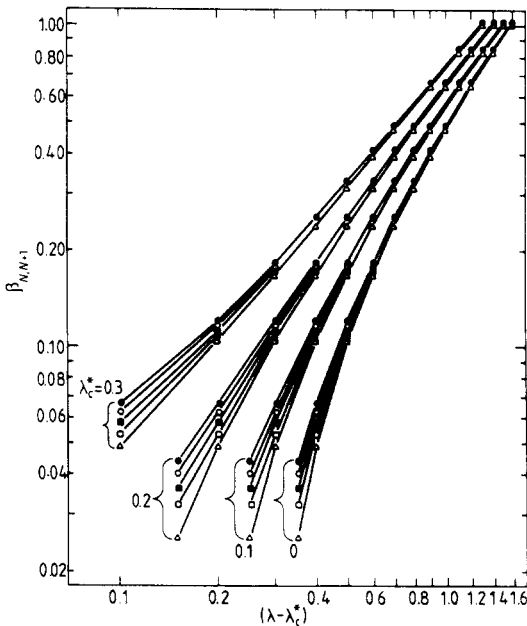


Figure 7. Function $\beta_{N,N+1}$ double-logarithmically plotted against $\lambda - \lambda_c^*$ for different λ_c^* and different chain lengths N . ($(N, N + 1) = 2, 3$ (Δ); $3, 4$ (\square); $4, 5$ (\blacksquare); $5, 6$ (\circ); $6, 7$ (\bullet).)

4. Conclusion

We find that the two-dimensional three-state Potts model with ferromagnetic interactions in one direction and antiferromagnetic interactions in the other direction has a

massless low-temperature behaviour in the anisotropic limit of strong ferromagnetic interaction, and using universality this should be valid also in the isotropic case. The transition point has an essential singularity with an exponent σ less than 0.9. As the coupling λ of the quantum Hamiltonian cannot be directly given in terms of the temperature, it is not possible to determine the transition temperature of the two-dimensional classical model with this method. But because of the strong finite size effects it cannot even be completely excluded that the massless region shrinks down to zero temperature; this is, however, not very likely if one considers figures 2, 3 and 4.

We note that our findings agree with those of other authors. Howes *et al* (1983) have considered the quantum version of a more general model, finding with series expansions $\lambda_c = 0.10 \pm_{0.03}^{0.10}$ assuming $\sigma = \frac{1}{2}$ for the special case of our model Ostlund (1981) and Yeomans and Selke (1982) studied the chiral clock model which for $\Delta = 1.5$ is our model; they also find the massless phase.

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