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LETTER TO THE EDITOR

Finite size scaling analysis of the dilute Baxter–Wu model

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Abstract. The finite size scaling method is used to study the critical properties of the spin-1 Baxter–Wu model as function of the fugacity, z, of the vacant (spin zero) sites. For $z = 0$, the thermal exponent converges very quickly to the (exact) value $y_t = 3/2$. For $z > 0$, y_t monotonically increases beyond the value 2. This increase is interpreted as indicating a first-order transition. Out of several possible renormalisation group flows, the results seem to favour the one in which the critical Baxter–Wu Hamiltonian flows to the fixed point of the 4-state Potts model, with the amplitude of the marginal operator equal to zero.

There has been considerable recent interest in phase transitions and critical behaviour of q-state Potts models in two dimensions (for an excellent review, see Wu 1981). This interest is motivated, on the one hand, by the availability of increasingly accurate experimental observations on physical systems (Bretz 1977, Tejwani *et al* 1980, Roelofs *et al* 1981) that exhibit transitions predicted to be in various Potts universality classes (Alexander 1975, Domany *et al* 1977). On the other hand, considerable theoretical progress has been achieved, ranging from exact results on Potts (Baxter 1973) and related (Baxter and Wu 1973, Baxter 1980) models, to conjectured relationships (den Nijs 1979, Burkhardt 1980, Nienhuis *et al* 1980a) between Potts and eight-vertex exponents. These conjectures have recently been substantiated by both analytic (Black and Emery 1981, Nienhuis 1981) and numerical (Nienhuis *et al* 1979, 1980b) work. In particular, the den Nijs conjecture has been extended to Potts tricritical exponents by Nienhuis *et al*, who also presented a mechanism that describes the manner in which the transition becomes first order for $q > q_c = 4$.

According to their picture, based on real space renormalisation group calculations, the critical and tricritical fixed points, when viewed as functions of continuous q, constitute two branches of the same function. As $q \to 4^-$, the two branches merge, implying the existence of a marginal operator for the $q = 4$ Potts model, giving rise to logarithmic corrections (Nauenberg and Scalapino (NS) 1980). This picture was obtained by viewing the q-state Potts models as a special subspace of more general $(q+1)$-state Potts lattice gas (PLG) models (Berker *et al* 1978) in which a site can be either in one of the q Potts states or 'vacant'.

The dilution operator, which controls the density of vacancies, plays a central role in the picture mentioned above; this is the operator which becomes marginal as $q \to 4$.

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Various calculations can be viewed as supporting this picture, and in particular, the existence of a marginal operator and logarithmic corrections for $q=4$. Herrmann (1981) has studied the quantum mechanical version of the model, and found explicitly the logarithmic corrections. Methods such as series analysis (Zwanzig and Ramshaw 1977), Monte Carlo renormalisation group (Eschbach *et al* 1981) and finite size scaling (Blöte *et al* 1981) which proved to yield the thermal exponent of various models with good accuracy and reasonably fast convergence, have failed to reproduce the expected value of $y_t = 3/2$ (or $\alpha = 2/3$). This can be viewed as a manifestation of slow convergence to the fixed point, and of logarithmic corrections that obscure the dominant behaviour.

An apparent difficulty with this picture is posed by the Baxter–Wu (Baxter and Wu (BW) 1973) model. This model is believed, on the basis of symmetry, to belong to the 4-state Potts universality class† (Domany and Riedel 1978). Indeed, the exact solution yields the value $\alpha = 2/3$ for the specific heat exponent, in agreement with the conjectured value (den Nijs 1979) for the 4-state Potts model. However, unlike the 4-state Potts model, the exact BW solution *does not contain logarithmic corrections.*

The aim of the present letter is to understand this apparent contradiction. In order to study this question, we generalise the BW model by introducing *annealed vacancies.* The Hamiltonian is thus written as

$$\bar{H} = -H/k_t T = K \sum_{\langle ijk \rangle} S_i S_j S_k + \Delta \sum_i (S_i^2 - 1) \tag{1}$$

where $S_i = 1, 0, -1$ and $\langle ijk \rangle$ denotes a triplet of nearest neighbour sites of a triangular lattice. The parameter $z = e^{-\Delta}$ represents the fugacity of the vacancies. The original spin-$\frac{1}{2}$ BW model is recovered in the limit $z = 0$. It is the addition of similar vacancies that enabled Nienhuis *et al* (1979) to find that the q-state Potts model becomes first order for $q > q_c$ (or for large z). As NS note, $\psi = z - z_c$ becomes marginal at the multi-critical point $q = q_c = 4$ and yields logarithmic corrections to the 4-state Potts model. In fact, NS conjectured that such corrections are absent in the BW model because it happens to have $\psi = 0$.

In general, we expect that the addition of vacancies will yield a critical line $K_c(z)$. The transition at $z = 0$ is second order (Baxter and Wu 1973). The transition at $T = 0$ is expected to be first order because of the clustering of occupied sites. One may thus expect a tricritical point at some intermediate point. *A priori*, there exist several possible renormalisation group (RG) scenarios by which the absence of logarithmic corrections in the BW model can be explained: (i) The BW and the 4-state Potts models might be described by completely orthogonal parameter spaces, with no RG flows relating them to each other. In this case, the critical surface of the BW model is indeed described by the single parameter z. If the tricritical point occurs at some finite value of z, then the fixed-point structure on the critical line would have to be described as in figure 1(a): the Hamiltonian flows to the critical fixed point (BWC) for small z, and to the discontinuity fixed point (D, $z = \infty$) for large z, the two regions being separated by the tricritical point (BWT). Note that the critical and tricritical points coincide in the case of the 4-state Potts model, yielding the logarithmic corrections in that case. The absence of such corrections in the exact solution of the BW model rules out the possibility that BWC and BWT coincide. (ii) There could exist an additional (unknown) parameter ϕ, which connects the BW model to the 4-state Potts model. In that case, the critical surface will become

† This was first pointed out by R B Griffiths.

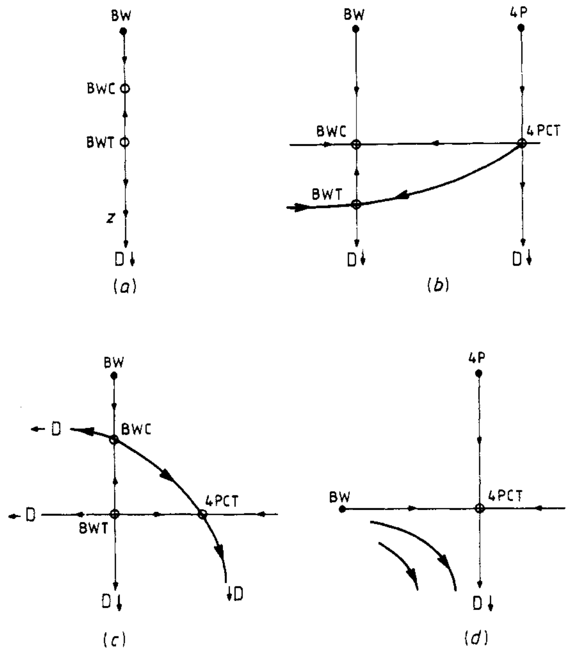

Figure 1. Possible renormalisation group flow scenarios for the BW model. BW = initial Baxter–Wu model Hamiltonian; BWC = BW critical fixed point; BWT = BW tricritical point; D = discontinuity fixed point; 4P = initial 4-state Potts model Hamiltonian; 4PCT = 4-state Potts fixed point.

two dimensional, and three possible flows are shown in figures 1(*b*), (*c*) and (*d*). The introduction of vacancies might change both z and ϕ, and have flows to the critical–tricritical 4-state Potts model fixed point, 4PCT, or to one of the BW fixed points mentioned above. Figure 1(*b*) describes a situation in which the 4PCT fixed point is unstable with respect to the operator leading to the BW model. As far as the BW model is concerned, the predictions remain as in scenario (*a*). (iii) Figure 1(*c*) describes the opposite situation, in which the 4PCT point is stable. If dilution moves the BW model to the right and down, then this picture implies a region of second order which is described by the 4PCT point (including logarithmic corrections). A first-order transition will result if dilution moves the BW model to the left. Note that although the BW and the 4-state Potts models have the same critical exponents, they are described in both figures 1(*b*) and 1(*c*) by two distinct fixed points. (iv) Finally, we could have only one fixed point, i.e. that of the 4-state Potts model 4PCT (figure 1(*d*)), that governs the critical behaviour of the BW model as well.

In order to decide which of these pictures is correct, we performed a finite size scaling analysis of the model (1) (Fisher and Barber 1972, Nightingale 1976). We obtained the critical coupling K_c and the thermal critical exponent y_t from the equation

$$\xi\left[t, \frac{1}{N}\right] = \frac{N}{N'}\xi\left[\left(\frac{N}{N'}\right)^{y_t} t, \frac{1}{N'}\right] \tag{2}$$

where $t = (K - K_c)/K_c$ and ξ is the correlation length of an infinite strip of width N and N' respectively, which is calculated exactly from the ratio of the two largest eigenvalues of the transfer matrix. Since our model equation (1) has three states per lattice site we had to find the largest eigenvalues of a $3^N \times 3^N$ transfer matrix T. This was done by writing T as a product of N sparse matrices and calculating the eigenvalues by numerical iteration (Nightingale 1976). K_c and y_t for fixed $z = e^{-\Delta}$ were obtained from equation (1) by calculating $\xi(t, 1/N)$ for two different strip widths N and N'. We used strips up to $N = 8$ with periodic boundary conditions which did not destroy the ground-state structures.

For the pure Baxter–Wu model ($z = 0$ in equation (1)), we obtained $K_c = 0.43938$, 0.44044 and $y_t = 1.504, 1.501$ for strips $N/N' = 4/6$ and 6/8, respectively, which agrees well with the exact result (Baxter and Wu 1973) $K_c = 0.44068$ and $y_t = 1.5$. The fast convergence with N confirms the absence of logarithmic corrections.

The results for the diluted case $z \neq 0$ are shown in figures 2 and 3. y_t strongly increases with z, to values much larger than $y = 2$. This result is obviously in contradiction with cases (i) and (ii). Experience with other tricritical points (Kinzel and Schick 1981) shows that in these cases we expect y_t to approach the pure value $y_t = 1.5$ for z less than the tricritical value z_t, and then to increase inside the first-order region.

The same reasoning implies that if figure 1(c) were correct, the addition of z causes the BW Hamiltonian to flow to the left-hand side of the picture, and not towards the 4PCT fixed point. On the other hand, the picture suggested by Nienhuis *et al* (1979) implies that vacancies move the 4-state Potts Hamiltonian downwards, through the 4PCT fixed point. It is difficult to visualise how these two directions of flow can coexist. Moreover, the possibility (iii) contains the unaesthetic feature of having two distinct fixed points for the two universally equivalent models. Although this picture is not completely ruled out, we find it very unlikely.

We are thus left with figure 1(d). We argue that our results are fully consistent with this picture. For $z = 0$ the BW model flows to the 4PCT fixed point, and therefore the two models exhibit the same exponents. As soon as $z > 0$, the dilute BW model flows to the

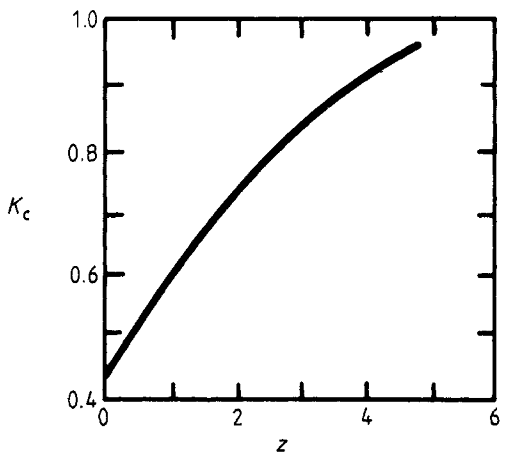

Figure 2. Dependence of K_c on z from finite size scaling.

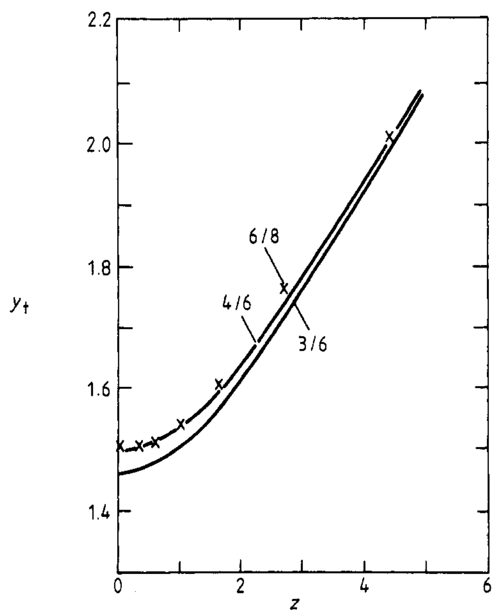

Figure 3. Dependence of y on z from several finite size strips.

D fixed point, implying a first-order transition. The fact that we find no finite range of z values in which the transition is second order implies that the BW initial Hamiltonian indeed occurs exactly on the separatrix line, on which the parameter ψ of NS is exactly zero.

Our conclusion is supported also by the following qualitative considerations. The (full lattice) BW model can be related to the dilute 4-state Potts model by a prefacing transformation (Berker *et al* 1978). The triangular lattice can be broken into interacting triangular cells with three Ising spins per cell. A cell has eight possible states, four of which [(+++), (+−−); (−+−), (−−+)] appear in one of the ground-state configurations of the BW model. Each of these states can be projected onto one of four equivalent Potts cell states, while the remaining four cell states, that are 'disordered', are projected onto a vacancy. Thus the model obtained after prefacing may correspond to a dilute 4-state Potts model with some additional irrelevant operators, and precisely the correct amount of dilution that corresponds to $\psi = 0$. Addition of vacancies to the BW model will obviously increase the amount of vacancies in the 4-state Potts model obtained by prefacing, thereby driving the transition immediately to first order. This picture also indicates a possible manner in which the BW model could be driven to the other side of the $\psi = 0$ line, i.e. introduction of interactions that will cause the four cell states that are projected onto a vacancy to be less suppressed. (This might be done by adding further neighbour interactions.) Such an operator, together with the dilution introduced above, may provide a way to drive the BW model to a continuous transition with logarithmic corrections. This possibility was not checked numerically, since introduction of further than nearest neighbour interaction necessitates working with two row to two row transfer matrices, which are too large to handle efficiently; however, Monte Carlo simulations of such models may be of use.

Unfortunately a theory of the behaviour of $\xi(t, 1/N)$ at a first-order transition is still missing. However, experience with other first-order transitions (Kinzel and Schick 1981, Blöte *et al* 1981) show that y_t increases as a function of parameters which change the transition from second to first order. y_t does not approach the value $y_t = 2$ which is predicted if the first-order transition is described by a discontinuity fixed point (Nienhuis and Nauenberg 1975), rather it takes values much larger than $y_t = 2$ inside the first-order region. We see the same behaviour in our model, figure 2. Thus we conclude that our results support the existence of a first-order transition for non-zero values of $z = e^{-\Delta}$, in agreement with the RG scenario of figure 1(d). The conjecture of NS, that both the 4-state Potts and the BW models are described by the same fixed point, thus finds some support.

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