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LETTER TO THE EDITOR

Duality of ordinary and extraordinary surface critical behaviour in the two-dimensional Potts model

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Abstract. The dual relationship between semi-infinite two-dimensional q-state Potts models with free and fixed spin boundary conditions is used to study the surface critical behaviour at the bulk critical temperature with fixed boundary spins, i.e. the extraordinary transition. Both the magnetisation and energy densities have singularities of the same form $|T-T_c|^{2-\alpha}$ as the bulk free energy. At $T=T_c$ both the spin-spin and energy-energy correlations decay as r^{-4} parallel to the surface.

Semi-infinite magnetic systems with ferromagnetic interactions and free surfaces exhibit several types of surface critical behaviour (Binder 1983) depending on the relative strengths of the surface and bulk coupling constants. If the surface spins order at the bulk critical temperature as the temperature is lowered, there is said to be 'ordinary' critical behaviour. If the spatial dimensionality of the surface exceeds a lower critical value and the surface couplings are sufficiently enhanced, the surface spins order at a critical temperature above the bulk critical temperature in a transition known as the 'surface' transition. As the temperature is then lowered through the bulk critical temperature, the 'extraordinary' transition takes place. Finally, if the surface couplings are just enhanced to the point that the critical temperatures for the bulk and surface transitions coincide, there is 'special' or 'multicritical' surface behaviour.

The extraordinary transition, in which the bulk orders in the presence of a spontaneous surface magnetisation, is thought to be equivalent to the ordinary transition in the presence of a surface magnetic field (Bray and Moore 1977). In the semi-infinite two-dimensional Potts model the boundary dimension is too low to support a spontaneous surface magnetisation above the bulk critical temperature, and a surface field is essential for extraordinary critical behaviour. In this letter the extreme case of boundary spins locked rigidly in the same state, e.g. by an infinite surface field or by infinite edge couplings, is considered.

The ordinary and special transitions have been investigated theoretically in considerable detail with the ε expansion (Diehl 1982) and other methods (Binder 1983, Cardy 1984a). The surface transition belongs to the same universality class as the $(d-1)$-dimensional bulk transition and thus is also considered to be well understood theoretically. The extraordinary transition has been studied to a lesser extent than the ordinary, special and surface transitions. Bray and Moore (1977) have developed a scaling theory for the extraordinary transition that has not been checked very generally, for

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example with the ε expansion. However, it agrees with exact results for the two-dimensional Ising model with a surface field (McCoy and Wu 1973) and, apart from minor discrepancies, with recent calculations for the n-vector model in the large-n limit (Ohno and Okabe 1984).

In this letter exact results are obtained for the surface critical behaviour of the two-dimensional semi-infinite q-state Potts model with fixed boundary spins and compared with the scaling theory of Bray and Moore for the extraordinary transition. The derivation makes use of a standard duality transformation (Syozi 1972), which replaces free spin boundary conditions by fixed boundary spins (Cardy 1984b), to translate known results for the ordinary transition into results for the extraordinary transition. The surface magnetisation and surface energy density are found to have leading thermal singularities $|T-T_c|^{2-\alpha}$ at the extraordinary transition. Here α is the standard bulk critical exponent (Stanley 1971). At $T=T_c$ both the spin-spin and energy-energy correlations decay as r^{-4} parallel to the surface. The results for the magnetisation and spin-spin correlation function agree with the predictions of Bray and Moore (1977). These authors do not discuss the energy density. However, it is argued below that the magnetisation and energy densities have the same extraordinary critical behaviour, in general.

Consider a two-dimensional q-state Potts model on a square lattice of N sites with homogeneous nearest-neighbour couplings $K=J/k_BT=\ln(x+1)$. The partition function is given by

$$Z_N(x)=\sum_{s_1=0}^{q-1}\cdots\sum_{s_N=0}^{q-1}\prod_{\langle ij\rangle}[1+x\delta^{(q)}(s_i-s_j)]. \tag{1}$$

Here $\delta^{(q)}(s)$ is a Kronecker delta of modulus q. It equals 1 if $s=0, \pm q, \pm 2q, \ldots$, and vanishes otherwise.

A convenient method for deriving duality relations for the Potts model is outlined in Knops (1977) and Burkhardt (1979). Since the summand in (1) involves relative spin variables $s_{ij}=s_i-s_j$, one converts the sum over N site variables s_i in (1) to a sum over $2N$ bond variables s_{ij}. The bond variables are not all independent, but satisfy a constraint of the form $s_{12}+s_{23}+s_{34}+s_{41}=0$ around each of the N elementary squares of the lattice. One may sum over the s_{ij} independently after inserting a Kronecker delta in the form

$$\delta^{(q)}(s_{12}+s_{23}+s_{34}+s_{41})=\frac{1}{q}\sum_{t=0}^{q-1}\exp\left(\frac{2\pi \mathrm{i}}{q}(s_{12}+s_{23}+s_{34}+s_{41})t\right) \tag{2}$$

for each square into the summand in (1). The only part of the partition sum that involves a particular bond variable s_{ij} is given by

$$\frac{1}{\sqrt{q}}\sum_{s_{ij}=0}^{q-1}[1+x\delta^{(q)}(s_{ij})]\exp\left(\frac{2\pi \mathrm{i}}{q}s_{ij}(t_k-t_l)\right)=(x/\sqrt{q})[1+(q/x)\delta^{(q)}(t_k-t_l)]. \tag{3}$$

From (1) and (3) one sees that the variables t_k and t_l, which come from the Kronecker deltas (2) associated with the two squares separated by the bond with bond variable s_{ij}, may be interpreted as site variables of a dual Potts model with couplings $x^*=q/x$. In the large-N limit, in which boundary effects are negligible, $Z_N(x)=(x^2/q)^N Z_N(q/x)$. The criticality condition is clearly $x_c=\sqrt{q}$.

In applying the duality transformation to the semi-infinite Potts model with a free surface, it is useful to think of an infinite lattice of Potts spins with vanishing bonds $(x=0)$ in one half-space and non-vanishing bonds in the other. Since the vanishing bonds transform into infinite bonds under $x^*=q/x$, $x=\exp(K)-1$, the duality transformation replaces the Potts model with a free surface by a Potts model with boundary spins locked in the same state by infinite edge couplings.

To determine the dual transformation properties of the nearest-neighbour correlation function or energy density $\langle\delta^{(q)}(s_{ij})\rangle$, we insert a factor $\delta^{(q)}(s_{ij})$ into the summand in (3) and obtain

$$\frac{1}{\sqrt{q}}\sum_{s_{ij}=0}^{q-1}[1+x\delta^{(q)}(s_{ij})]\delta^{(q)}(s_{ij})\exp\left(\frac{2\pi i}{q}s_{ij}(t_k-t_l)\right)=(1/\sqrt{q})(1+x). \qquad (4)$$

Dividing equation (4) by (3) leads to the result

$$\frac{x}{1+x}\langle\delta^{(q)}(s_{ij})\rangle+\frac{x^*}{1+x^*}\langle\delta^{(q)}(t_{kl})\rangle^*=1. \qquad (5)$$

Similarly one finds that the energy-energy correlation function transforms according to

$$\left(\frac{x}{1+x}\right)^2[\langle\delta^{(q)}(s_{ij})\delta^{(q)}(s_{i'j'})\rangle-\langle\delta^{(q)}(s_{ij})\rangle\langle\delta^{(q)}(s_{i'j'})\rangle]$$
$$=\left(\frac{x^*}{1+x^*}\right)^2[\langle\delta^{(q)}(t_{kl})\delta^{(q)}(t_{k'l'})\rangle^*-\langle\delta^{(q)}(t_{kl})\rangle^*\langle\delta^{(q)}(t_{k'l'})\rangle^*]. \qquad (6)$$

Here i,j and i',j' denote pairs of nearest-neighbour sites, and k,l and k',l' the corresponding nearest-neighbour pairs on the dual lattice.

Equations (5) and (6) are clearly invariant under interchange of the original system and the dual system. In this letter the unstarred thermal averages and spin variables s always refer to the system with free boundaries and ordinary surface critical behaviour, indicated by broken lines in figure 1. The starred system with variables t, which has infinite boundary couplings and extraordinary critical behaviour, is indicated by full lines in figure 1, with a double line at the boundary.

Cardy (1984a) has shown that the energy-energy correlation function decays with separation r as r^{-4} parallel to the boundary at criticality in the ordinary transition of the two-dimensional semi-infinite Potts model. The r^{-4} decay is consistent† with a thermal singularity of the form $|T-T_c|^{2-\alpha}$ in the surface energy density‡ at the ordinary transition. The duality relations (5) and (6) immediately imply that in the extraordinary transition there is also a $|T-T_c|^{2-\alpha}$ singularity in the surface energy density and an r^{-4} decay of energy-energy correlations parallel to the surface.

Thus far the critical behaviour of the energy density and energy-energy correlations has been studied in a Potts model with infinite boundary couplings that lock all the boundary spins in the same state t_b. In the starred thermal averages, t_b is summed over the values $0, 1, \ldots, q-1$. In discussing the critical behaviour of the order parameter, it is appropriate to consider an infinite surface field that breaks the symmetry in the q possibilities for t_b and fixes all the surface spins in one particular state. Both boundary conditions clearly give identical results for non-symmetry breaking quantities such as the energy density and the energy-energy correlation function.

† The scaling ansatz $\varepsilon_s(\boldsymbol{r},t)=b^{-x_s}\varepsilon_s(\boldsymbol{r}/b, b^{1/\nu}t)$, $t=T-T_c$ for the surface energy density in thermal averages and the hyperscaling relation $2-\alpha=d\nu$ imply $\langle\varepsilon_s\rangle\sim t^{x_s\nu}t^{(2-\alpha)x_s/d}$, $\langle\varepsilon_s(\boldsymbol{r})\varepsilon_s(0)\rangle-\langle\varepsilon_s\rangle^2\sim r^{-2x_s}$ at $t=0$. The results for the ordinary transition of the two-dimensional Potts model correspond to $x_s=d=2$.

‡ That the leading thermal singularity in the surface energy density has the form $|T-T_c|^{2-\alpha}$ was established for the ordinary transition of the n-vector model to all orders in $\varepsilon=4-d$ by Dietrich and Diehl (1981).

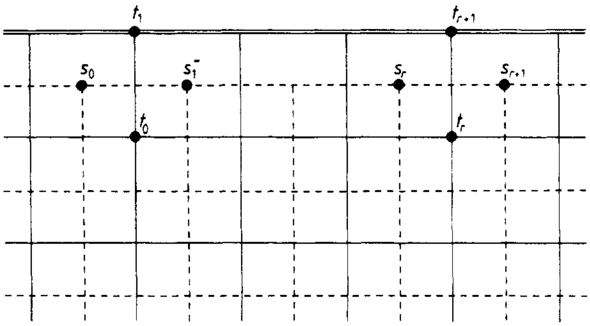

Figure 1. The lattice of spins s_i with couplings K (broken lines) and free boundary conditions. The lattice of dual spins t_k with interior couplings K^* (full lines) and infinite boundary couplings (double full lines).

The local order parameter or magnetisation $m_k^{(\alpha)}$ at lattice site k may be defined as

$$m_k^{(\alpha)} = \langle \delta^{(q)}(t_k - \alpha) \rangle_{t_b} - q^{-1} \tag{7}$$

where the thermal average is taken with the boundary spins fixed in state t_b. Since $\Sigma_\alpha m_k^{(\alpha)} = 0$ and the $q-1$ components $m_k^{(\alpha)}$ with $\alpha = t_b + 1, t_b + 2, \ldots, t_b + q - 1$ are all the same, the order parameter is entirely determined by the probability $\langle \delta^{(q)}(t_k - t_b) \rangle_{t_b}$ that spin k is in the same state t_b as all the boundary spins. Since this probability is independent of the particular value of t_b, one has

$$\langle \delta^{(q)}(t_k - t_b) \rangle_{t_b} = \langle \delta^{(q)}(t_k - t_b) \rangle^* \tag{8}$$

where the star denotes the thermal average considered above, with infinite surface couplings and no symmetry-breaking field. Thus the extraordinary critical behaviour of the order parameter is determined by the correlation function on the right side of (8), which is related by duality to a correlation function with ordinary critical behaviour.

The critical behaviour of the correlation function on the right side of (8) is particularly clear in the case in which spin t_k is one lattice constant from the boundary, like spin t_0 in figure 1. In this case the correlation function is just the energy density, a quantity we have already considered. Since one expects the same universal critical behaviour at sites $1, 2, 3, \ldots$ lattice constants from the boundary, we conclude that the order parameter, like the energy density, has a thermal singularity of the form $|T - T_c|^{2-\alpha}$ at the extraordinary transition. This result is in agreement with the scaling prediction of Bray and Moore (1977) for the order parameter.

The argument just given, according to which the order parameter and the energy density have the same extraordinary critical behaviour, can be readily extended to other spin systems in arbitrary dimension. Consider, for example, the classical n-vector model with spins $\boldsymbol{S}$ of unit length and an infinite surface field h_1 in the z direction. It is clear that $\langle S_k^z \rangle = \langle \boldsymbol{S}_k \cdot \boldsymbol{S}_b \rangle$, where spin b is on the boundary. In a finite field h_1 the two thermal averages are no longer equal, but the universal critical behaviour of each is presumably unchanged. In the extraordinary transition a spontaneous surface magnetisation or an applied surface field breaks the rotational symmetry, and the distinction between local operators with the symmetry of the magnetisation density and the energy density disappears.

The heuristic argument just given suggests that in the extraordinary transition of the two-dimensional Potts model, the spin–spin correlation function decays as r^{-4}

parallel to the surface, as we have already established for energy-energy correlations. A similar conclusion follows from the dual transformation properties of the spin-spin correlation function, which we now consider.

In the case of spin-spin correlations it is clear that ensemble averages with boundary spins coupled by an infinite interaction constant or with boundary spins fixed in one particular state are the same. To simplify the discussion, let us consider the correlations of spins t_0 and t_r located one lattice constant from the boundary and separated by r lattice constants, as shown in figure 1. Using the Fourier representation of the Kronecker delta (2) and recalling that the boundary spins t_1 and t_{r+1} (see figure 1) are always in the same state because of the infinite interaction constant at the boundary, one has

$$\langle\delta^{(q)}(t_0-t_r)\rangle^* = \frac{1}{q}\sum_{\nu=0}^{q-1}\left\langle \exp\left(\frac{2\pi \mathrm{i}}{q}(t_0-t_1+t_{r+1}-t_r)\nu\right)\right\rangle^*. \qquad (9)$$

Since the quantity in angular brackets on the right side of (9) only involves relative nearest-neighbour spin variables t_0-t_1 and t_r-t_{r+1}, it is straightforward to rewrite it in terms of correlation functions of the dual system. Converting sums over site variables t_k to sums over bond variables t_{kl} as discussed below equation (1), one obtains

$$\begin{aligned}\langle\delta^{(q)}(t_0-t_r)\rangle_c^* &= x^2(1-q^{-1}x^2)(1+x)^{-2}\langle\delta^{(q)}(s_0-s_1)\delta^{(q)}(s_r-s_{r+1})\rangle_c \\ &\quad + q^{-1}x^2\sum_{\nu=0}^{q-1}\langle\delta^{(q)}(s_0-s_1+\nu)\delta^{(q)}(s_r-s_{r+1}-\nu)\rangle_c. \end{aligned} \qquad (10)$$

Here the subscript c denotes the unsubscripted average minus its limit as $r\to\infty$. The dual spins s_0, s_1, s_r, s_{r+1} are located on the boundary of the system with free-spin boundary conditions, as shown in figure 1.

The first correlation function on the right side of (10) is the energy-energy correlation function, which decays as r^{-4} parallel to the surface in the ordinary transition, as discussed above. Since $\langle\delta^{(q)}(s_0-s_1+\nu)\rangle = (q-1)^{-1}(1-\langle\delta(s_0-s_1)\rangle)$ for $\nu = 1, 2, \ldots, q-1$, all the other correlation functions on the right side of (10) are essentially energy-energy correlation functions and are also expected (see the first footnote) to fall off as r^{-4}. Thus we conclude that the left side of equation (10), i.e. the spin-spin correlation function of the semi-infinite Potts model with fixed boundary spins, also decays as r^{-4} at criticality. This result agrees with the general scaling prediction r^{-2d}, d being the spatial dimension, of Bray and Moore (1977) for the extraordinary transition.

The dual relationship between Potts models with free and fixed spin boundary conditions determines the universal amplitude $A = \lim \xi(L, T_c)/L$, $L\to\infty$ of the correlation length $\xi(L, T)$ in strips of finite width L and infinite length with fixed boundary spins at the bulk two-dimensional critical temperature. With a general argument based on conformal invariance, Cardy (1984c) has shown that $A=(2\pi x)^{-1}$ for periodic boundary conditions and $A=(\pi x_s)^{-1}$ for free boundaries. In the case of spin-spin correlations $x=\eta/2$ and $x_s=\eta_\parallel/2$, where η and $\eta_\parallel$ are standard bulk and surface critical exponents (Stanley 1971, Binder 1983). For energy-energy correlations $x = d-\nu^{-1} = d(1-\alpha)/(2-\alpha)$, where α and ν are also standard bulk exponents, and $x_s = d = 2$ (Nightingale and Blöte 1983, Cardy 1984a, Burkhardt and Guim 1985). Since both spin-spin and energy-energy correlations in Potts strips with fixed boundary spins correspond to energy-energy correlations with free boundary spins, we predict

$A=(2\pi)^{-1}$ for either spin-spin or energy-energy correlations in Potts strips with fixed boundary spins.

The results for the Potts model reported here agree with the scaling predictions of Bray and Moore (1977) for the extraordinary transition. Cardy (1984a) has shown that conformal invariance determines the ordinary surface critical behaviour of a large class of two-dimensional systems, and it would be interesting to extend this approach to the extraordinary transition†. Finally, results within the ε expansion (Diehl 1982) for the extraordinary transition of the n-vector model would also provide a useful check of the scaling theory.

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† J L Cardy (private communication) has calculated the spin-spin correlation function of the two-dimensional Ising model at the extraordinary transition with the conformal-invariance approach. The result is the same as equation (4.23) of Cardy (1984a) except that the minus sign is replaced by a plus sign. The correlation function decays as r^{-4} parallel to the surface, in agreement with the results of this letter.