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LETTER TO THE EDITOR

Defect free energies of Potts models on hierarchical lattices

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Abstract. The excess defect free energies of interface-like defects in Potts models on hierarchical lattices are calculated exactly. For $q = 2$ (Ising model) the depinning transition takes place. For $q > 2$ the free energies show anomalies which may be interpreted as the intrusion of the non-boundary phase into the interphase region, in agreement with recent Monte Carlo simulations.

The structure of an interface in systems like the Ising model, in which only *two* ordered phases coexist below the critical temperature T_c, is by now reasonably well understood (Widom 1972, Abraham 1980, Pandit *et al* 1982). However, the behaviour of an interface in e.g. the Potts model (Potts 1952, Wu 1982), in which more than two phases coexist, is less well understood. Only quite recently Selke and Pesch (1982) have used Monte Carlo simulation to analyse the interface in the $d = 2$, $q = 3$ state Potts model. They showed that, when the interface between two phases (e.g. phases '1' and '2') is created using suitable boundary conditions, then the phase '3' intrudes into the interphase region at sufficiently high temperature, quite close to the critical temperature T_c. A similar phenomenon was also observed by Kinzel (1982) who analysed the interface in the $d = 1$, q-state Potts model. In this note we present the exact calculation of excess defect thermodynamic functions for the general q-state Potts model on a suitably defined hierarchical lattice. These functions exhibit a remarkable richness of behaviour, and some of their features are suggestive of phenomena observed on two-dimensional lattices (Selke and Pesch 1982).

Hierarchical lattices have been a subject of considerable recent interest (Kaufman and Griffiths 1981, 1982, Griffiths and Kaufman 1982) due to the fact that the Migdal–Kadanoff recursion relations, approximate for the Ising square lattice, are exact for hierarchical lattices (Berker and Ostlund 1979). The specific hierarchical lattice we use is constructed in the way indicated in figure 1. Figure 1(a) shows the iteration procedure for 'regular' (non-defect) bonds and figure 1(b) the iteration procedure for defect bonds. When the two are combined the lattice in figure 1(c) is obtained. This process is then iterated *ad infinitum*. Defect bonds have strength K_1, regular bonds K, and we shall take $K_1 = aK$, where a is some arbitrary parameter. The Potts model Hamiltonian (Wu 1982) is of the general form

$$-\beta\mathcal{H} = H = NK_0 + \sum_{\langle ij \rangle} K_{ij}(2\delta_{S_iS_j} - 1) \tag{1}$$

where nearest-neighbour $\langle ij \rangle$ spins S_i and S_j interact via K_{ij}. Every site in the lattice

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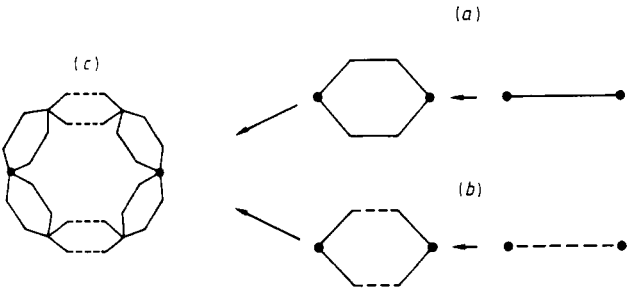

Figure 1. Construction of hierarchical lattice: (*a*) iteration procedure for non-defect bonds; (*b*) iteration procedure for defect bonds; (*c*) the resulting lattice.

is assigned the spin-independent term K_0 (there are N sites) which will be needed for calculation of thermodynamic functions. The Hamiltonian in equation (1) is defined in such a way that negative couplings K_{ij} will favour spins of different 'orientation'. The total, dimensionless, free energy in the thermodynamic limit is of the form

$$F_N = \mathrm{Tr}_{[S]}\, \mathrm{e}^{H} = Nf_\mathrm{b} + N_\mathrm{d} f_\mathrm{d} + \ldots \tag{2}$$

where dots indicate terms diverging less rapidly than N_d, f_b is the bulk free energy density, N_d the number of defect sites and f_d the excess defect free energy density. Note that f_d will be a function of both K and K_1, while f_b depends only on K. The trace in equation (2) is taken over all spin configurations $[S]$. Applying the usual renormalisation group procedure (Niemeijer and van Leeuwen 1976), the renormalised couplings K' and K_1' will be related to the original ones via recursion relations, the new system will have a total of $N' = b^{-d}N$ sites and $N_\mathrm{d}' = N_\mathrm{d}/2$ defect sites. However, the total free energy will not change. Thus

$$F_N = F_{N'} = N' f_\mathrm{b}(K') + N_\mathrm{d}' f_\mathrm{d}(K', K_1') + \ldots \tag{3}$$

where the dependence on couplings is explicitly indicated. Comparing equations (2) and (3), we get the *scaling relation*

$$f_\mathrm{d}(K, K_1) = \tfrac{1}{2} f_\mathrm{d}(K', K_1'). \tag{4}$$

The spin-independent term K_0 will also change under renormalisation transformation: K_0' will be a function of K only for those spins which are connected with all non-defect bonds, and a function of both K and K_1 for spins connected with defect bonds. We shall distinguish the two as K_0' and K_{01}', respectively. Using definition equation (2) and scaling equation (4) we get (Švrakić and Wortis 1977)

$$f_\mathrm{d}(K, K_1) = \sum_{n=0}^{M-1} 2^{-(n+1)}(K_{01}^{(n)} - K_0^{(n)}) + 2^{-M} f_\mathrm{d}(K^{(M)}, K_1^{(M)}) \tag{5}$$

where n denotes the number of renormalisation group iterations. The strategy is clear: one iterates away from 'difficult' values of couplings K and K_1 into a region $(K^{(M)}, K_1^{(M)})$ where $f_\mathrm{d}(K^{(M)}, K_1^{(M)})$ can be easily calculated. The incremental defect free energy contributions (terms under summation sign), properly scaled, are collected in the process. Then $f_\mathrm{d}(K, K_1)$ immediately follows from equation (5).

In figure 2 we show the results of this calculation for the case $q = 2$ (Ising model). The defect free energies f_d are plotted for several values of the parameter a. It can

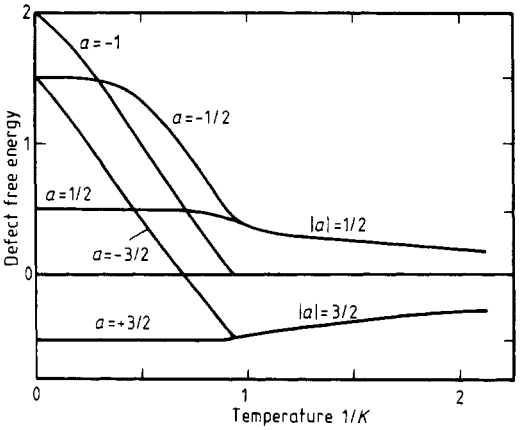

Figure 2. Excess defect free energies for $q=2$ (Ising spins). $f_d(a=-1)$ is the interface tension. For further details see text.

be seen that, when $a=-1$, the defect free energy vanishes at and above the (dimensionless) critical temperature $T_c=1/K_c$. This illustrates the fact that value $a=-1$ has a special meaning for the Ising model: $f_d(a=-1)$ is the interface tension. When $-1<a\leqslant 0$, and we show the case $a=-\frac{1}{2}$, the second derivative of the defect free energy (and this is proportional to the defect specific heat) will change sign at some temperature below the critical temperature T_c, signalling the onset of the wetting transition (Abraham 1980). The case $-1\leqslant a\leqslant 0$ corresponds to the interface-pinning defect, since one can show that such a defect in a hierarchical lattice with periodic boundary conditions is equivalent to the defect $0\leqslant a\leqslant 1$ in the lattice with antiperiodic boundary conditions. In particular, the calculated defect free energies will be the same, as seen in equation (5). Furthermore, this lattice cannot distinguish whether the defect is on the boundary or not, and this is reflected in the recursion relations (Kaufman and Griffiths 1982). This is generally not true in the two-dimensional Ising model since there it is important that the defect is located at the boundary (Abraham 1980) if the wetting (depinning) transition is to occur.

The vanishing of the $f_d(a=-1)$ above T_c in the Ising model is associated with cancellation of terms in equation (5), and this, in turn, happens because the initial relation $K_1=-K$ is preserved under iterations, i.e. $K_1^{(n)}=-K^{(n)}$. However, this relation is not preserved in the $q\neq 2$ Potts model because these systems do not possess ferromagnetic–antiferromagnetic symmetry. Therefore, if $f_d(a=-1)$ is calculated for $q\neq 2$, this quantity will not be the interface tension. In particular, this free energy will not vanish at the critical temperature $T_c(q)$. The limiting form for f_d when $K\to 0$ is given by $f_d/K\sim(1-a)(q-2)/q$, which is zero only if $a=1$ and/or $q=2$. This form is also valid for two-dimensional lattices and can be easily derived from the high-temperature expansion (Wu 1982). Figure 3 shows our results for $f_d(q)$ when $a=-1$ for a range of q-values. Several features are readily apparent. First, the critical temperature $T_c(q)$ will decrease with increasing values of q. For the lattice on figure 1(*c*), $T_c(q)=1/K_c$ is obtained as the solution of

$$2q=(e^{2K_c}-1)[(4e^{K_c}+1)^{1/2}-3]. \tag{6}$$

For the pair (K_c, q) satisfying equation (6) the defect coupling fixed point is given as

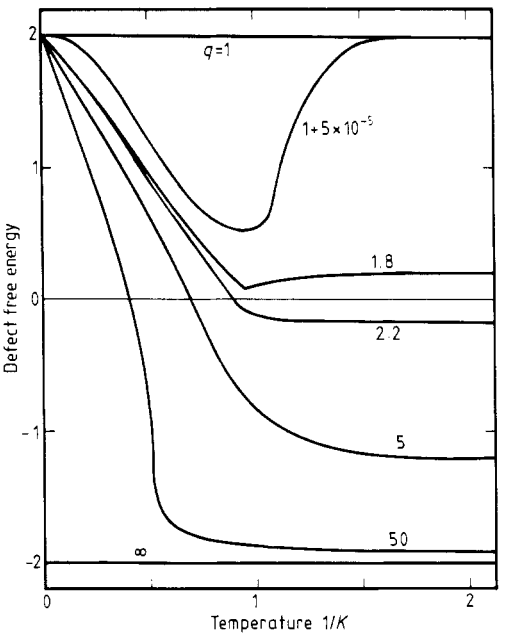

Figure 3. Excess defect free energies for $q \neq 2$ and $a = -1$.

$K_1^* = -K_c + \ln(q-1)$, clearly displaying the symmetry $K_1^{(n)} = -K^{(n)}$ when $q = 2$. Second, when $q = 1$, which corresponds to the percolation limit (Wu 1982), $f_d(q=1) = -2K$ for all values of K, indicating that there is no entropy associated with the defect in a system with only one phase (simply, such systems cannot be disordered). But the effect of increasing q slightly above 1, and we show the case $q = 1 + 5 \times 10^{-5}$, is quite impressive. Clearly, the insertion of negative coupling(s) in the Potts model can have a large effect depending on the value of q. At the other end of this behaviour is the $q \to \infty$ limit which has the high-temperature behaviour for all temperatures.

The behaviour of the defect free energies for the intermediate q-values is in between the above two extremes. As is seen in figure 3, $f_d(q > 2)$ will go through zero at some temperature $T_0(q)$ which is strictly lower than the critical temperature $T_c(q)$. The difference $T_c(q) - T_0(q)$ will stay relatively small when q is increased and will not appreciably change. *If* the interpretation is that $T_0(q)$ is the temperature at which the intrusion of other phases takes place (the defect is interface promoting), then our results suggest, in accordance with the exact results of Kinzel (1982), that such an intrusion will take place at temperatures which are close to the critical temperature. This is consistent with the Monte Carlo data of Selke and Pesch (1982). Furthermore, one expects the size of the intruding phase to be of the order of the correlation length and, if the above interpretation is accepted, then the boundary phase would play the role of the substrate and the intruding phase the role of the adsorbate exhibiting the wetting transition. This point clearly deserves further investigation, which is under way.

In summary, we have calculated excess defect free energies in Potts models on hierarchical lattices. In the case $q = 2$ (Ising model) suitably introduced defects give rise to the interface depinning transition, in agreement with the $d = 2$ result of Abraham

(1980). When $q \neq 2$ the observed anomaly (vanishing) of the free energy may suggest the intrusion of the non-boundary phase into the interphase region, as seen in recent Monte Carlo experiments (Selke and Pesch 1982).

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Note added. After this work was completed we learned that very recent Monte Carlo results (Selke 1982) performed on the $q = 4$ Potts model in two dimensions also show the intrusion of the non-boundary phase into the interphase region. This intrusion takes place at a temperature quite close to the critical temperature, in agreement with the results of this work. I am grateful to W Selke for this information.

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