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LETTER TO THE EDITOR

Variational renormalisation-group approach to the q-state Potts model in two dimensions

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Abstract. The two-dimensional q-state Potts model is investigated by means of a Kadanoff lower-bound renormalisation-group transformation that utilises a recent suggestion to identify disordered cells with vacancies. The topology of the phase diagram is obtained, including first- and second-order transitions for $q > q_c$ and $q \leq q_c$, respectively, as well as accurate results for critical and tricritical exponents and the critical value q_c.

Recently, Nienhuis *et al* (1979) presented the first renormalisation-group calculation for the two-dimensional q-state Potts model that yielded, with increasing q, the changeover in the phase transition from second to first order that this model is known to possess (Baxter 1973). The calculation employed a generalised Niemeijer–van Leeuwen (1976) transformation. The results were not completely satisfactory in that they depended on the choice of parameters in the weight function for which there was little guidance *ab initio*. The purpose of this Letter is to report work using Kadanoff's lower-bound renormalisation-group method, in which a variational principle is used to determine an optimal weight function depending on three variational parameters. First, the calculation reproduces the topology of the renormalisation-group phase diagram of the Potts model obtained earlier. Second, the calculations yield, for the critical value of q, $q_c \approx 4{\cdot}08$ in excellent agreement with Baxter's result $q_c = 4$. Third, the approach yields results for critical and tricritical exponents that provide strong support for a recent conjecture that relates the thermal exponents of the Potts and eight-vertex models.

The new concept introduced into the renormalisation-group treatment of the Potts model by Nienhuis *et al* (1979) is to allow the Potts model to develop vacancies as it is renormalised. In contrast to a majority rule mapping, disordered configurations of spins are assigned to the empty state or vacancy. This necessitates enlarging the space of Hamiltonians to that of the Potts lattice gas (PLG). The nearest-neighbour Hamiltonian is

$$-\beta\mathcal{H} = \sum_{\langle i,j \rangle} t_i t_j (K + J\delta_{s_i,s_j}) - \Delta \sum_i t_i, \tag{1}$$

where the first summation is over all nearest-neighbour pairs on a lattice. The lattice-gas variable t_i assumes the value one if there is a Potts spin $s_i = 1, 2, \ldots, q$ at lattice site i and zero otherwise. The couplings K and J denote lattice gas and Potts interaction parameters, and the chemical potential Δ governs the concentration of vacancies. The pure Potts model is recovered for $\Delta = -\infty$ or, equivalently, $K = \infty$. The

Hamiltonian describes for $q = 1$ the Ising lattice-gas and for $q = 2$ the Blume–Emery–Griffiths model.

The Kadanoff renormalisation-group transformation applied here is a straightforward generalisation of that described by Kadanoff (1975) and others (Burkhardt 1976, Dasgupta 1977). We consider a square lattice and a PLG Hamiltonian that can be written as a sum over elementary squares, $-\beta\mathcal{H} = \Sigma H_{SQ}$. We assume H_{SQ} to be invariant under interchange of any two sites on the square because the nearest-neighbour Potts Hamiltonian can be mapped onto this subspace by an exact decimation transformation (Kadanoff and Houghton 1975). This subspace involves twelve coupling constants K associated with the twelve possible spin configurations of a square. We use the weight function employed by Burkhardt (1976) for the Blume–Emery–Griffiths model. It maps a configuration $\{t_i, s_i\}$ of a square to t', s' with weight

$$W(t', s'; \{t_i, s_i\}) = N(\{t_i, s_i\}) \exp\left(t' \sum_{i=1}^{4} (p_1 t_i + p_2 t_i \delta_{s's_i} + p_3)\right) \tag{2}$$

where p_1, p_2, p_3 are variational parameters and $N(\{t_i, s_i\})$ is a normalisation factor such that $\Sigma_{t's'} W = 1$. As usual the Kadanoff approximation provides a lower bound to the free energy. The variational parameters employed to maximise this lower bound are determined at the fixed points of the recursion relations by applying the criterion that the free energy be stationary with respect to variation of the p_i (Kadanoff *et al* 1976). By investigating the behaviour of the free energy in the vicinity of each fixed point, we eliminate the solutions that correspond to minima or saddle points.

The calculation reproduces the topology of the renormalisation-group flow obtained by Nienhuis *et al* (1979) for the q-state Potts model and, in addition, it yields very accurate results for critical and tricritical exponents as well as the critical value q_c. For $q < q_c$, the recursion relations exhibit critical, tricritical and discontinuity fixed points. The critical fixed point attracts renormalisation-group flows commencing at the critical temperature of the pure Potts model. As q is increased, the critical and tricritical fixed points approach each other and annihilate at a critical value q_c. For $q > q_c$, only the discontinuity fixed point associated with a first-order transition (Nienhuis and Nauenberg 1975) remains. Therefore, the phase transition of the two-dimensional Potts model is continuous when $q \leqslant q_c$ and first-order when $q > q_c$. The approximate recursion relations yield $q_c \approx 4{\cdot}08$ in excellent agreement with the analytical result $q_c = 4$ of Baxter (1973).

The values of the three variational parameters p_1, p_2, p_3 at $q = 2$ are $(-3{\cdot}056, 5{\cdot}966, -1{\cdot}395)$ and $(-1{\cdot}146, 2{\cdot}190, -0{\cdot}217)$ for the critical and tricritical fixed points respectively, and for the discontinuity fixed point they approach infinity, approximately in the direction $(3, 1, -2)$. These fixed points agree with those found by Burkhardt (1976) for the Blume–Emery–Griffiths model. We have verified that the free energy, as a function of p_1, p_2, p_3, is a maximum at these three fixed points. The equations have an additional fixed-point solution in the pure Potts model subspace (p_1 and p_3 are infinite such that vacancies are excluded). That solution is identical to the one found by Dasgupta (1977), who did not consider the possibility of vacancies. It yields the erroneous result of a continuous phase transition for all q. Though this fixed point corresponds to a maximum of the free energy for variation of the parameter p_2 alone, in the larger parameter space p_1, p_2, p_3 it corresponds to a saddle point.

In figure 1, results for the critical and tricritical thermal exponent $y = \nu^{-1}$, as a function of q, are summarised and compared with a recent conjecture (den Nijs 1979,

Nienhuis *et al* 1979) that establishes a relation between the exponents of the Potts and eight-vertex (Baxter 1972) models,

$$(y-3)(y^{8v}-2)=3. \tag{3}$$

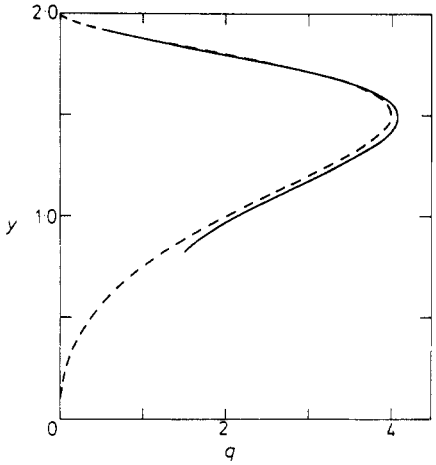

Figure 1. Critical and tricritical exponents (lower and upper branch, respectively) from the Kadanoff lower-bound approximation (solid curve) and the conjecture of den Nijs and Nienhuis *et al.*

Here $y^{8v}=(2/\pi)\cos^{-1}(\sqrt{q}/2)$ with $0\leqslant y^{8v}\leqslant 1$ along the critical branch and $-1\leqslant y^{8v}\leqslant 0$ along the tricritical branch of the curve. The numerical and conjectured data agree to within 0·2% for the tricritical and 3% for the critical exponents, with a larger deviation at the tip of the curve where the slope is infinite. Results for the tricritical exponents have been obtained independently by Burkhardt (1979, private communication). This excellent agreement provides strong support for the conjecture of equation (3). The results for the exponents reported here were calculated following the usual prescription of evaluating the derivative matrix of the interaction parameters K while keeping the variational parameters p constant (Kadanoff 1975, Kadanoff *et al* 1976). Although not in the full spirit of a variational calculation (Barber 1977, den Nijs and Knops 1978, van Saarloos *et al* 1978), this procedure yields exponents with a surprising accuracy for a number of systems. The calculation determines the spectrum of exponents for the space of twelve coupling constants. For the Ising case, $q=2$, we note that the leading (even) critical exponents 0·97, −0·94, −1·91, −2·93, ... are close to the set of integers 1, −1, −2, −3, ... The correction exponent −1 has recently been determined by Hamer *et al* (1979). The analysis of the transformation for those q not shown in figure 1 is less direct and will be reported elsewhere.

In summary, our variational calculation for the Potts model supports the basic idea of mapping disordered groups of spins to vacancies, confirms the renormalisation group topology reported previously, and strengthens the belief that the exponents of the Potts model are now known exactly.

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