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Q-state Potts models in Hamiltonian field theory for $Q \geqslant 4$ in (1+1) dimensions

C J Hamer

Department of Theoretical Physics, Research School of Physical Sciences, The Australian National University, Canberra, ACT 2600, Australia

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Abstract. Finite-lattice sequence extrapolation methods are applied to the Q-state Potts models in (1+1)-D Hamiltonian field theory. Thermal exponents $\nu = 0.71 \pm 0.02$, $\alpha = 0.53 \pm 0.02$ are obtained for the four-state model. Methods are discussed for treating the first-order transitions for $Q > 4$, and a sequence extrapolation is used to estimate the latent heat. Exact analytic formulae are derived for the ground-state energy, the mass gap, and the latent heat at the transition point; these are compared with the numerical results.

1. Introduction

In a recent paper (Hamer and Barber (1980), hereafter referred to as HB), a method was presented for accelerating the convergence of finite-lattice sequences to their bulk limit. The method employed a modification (Barber and Hamer 1980) of a sequence transformation due to Vanden Broeck and Schwartz (1979, hereafter VBS). Applied to the (1+1)-dimensional† Z_3 or three-state Potts model in a Hamiltonian field theory formulation, these techniques yielded estimates for the critical exponents of exkllent accuracy.

Here we apply the same techniques to Q-state Potts models with $Q \geqslant 4$, in (1+1) dimensions. This is a natural extension of the earlier work, and also allows us to explore the application of finite-size scaling methods to systems with a first-order phase transition.

Some properties of the Potts model have been derived analytically by Baxter (1973b). He has obtained expressions for the free energy at the critical point (where the model is self-dual), and shown that for $Q \leqslant 4$ the Q-state model undergoes a second-order transition, while for $Q > 4$ the transition becomes first-order, i.e. there is a finite latent heat. For $Q = 4$ the model is conjectured to have thermal exponents $\alpha = \nu = \frac{2}{3}$, $\alpha/\nu = 1$, on the basis of universality arguments (Enting 1975, Kadanoff 1977, Domany and Riedel 1978, den Nijs 1979).

Several numerical studies have been performed on these models. Restricting ourselves to the thermal exponents only, series analyses for $Q = 4$ have been made by Enting (1975) and Ditzian and Kadanoff (1979). A large number of renormalisation group analyses have been made, as listed by Hu (1980) and Black and Emery (1981). Recently, finite-size scaling treatments akin to the present one have been presented by Roomany and Wyld (1980b), Nightingale and Blöte (1980) and Blöte *et al* (1980). The

† That is, one space and one time dimension.

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last-named reference uses methods almost identical to ours, in a statistical mechanics (Euclidean space) framework.

The first objective addressed in this paper is to translate the known exact results of Baxter (1973b) and others into the Hamiltonian field theory framework. First, an equivalence is shown between the Potts model and a staggered eight-vertex model (Temperley and Lieb 1971, Baxter 1973b). The eight-vertex Hamiltonian is found by the transfer matrix procedure of Fradkin and Susskind (1978): at the self-dual point, it reduces to a Heisenberg–Ising Hamiltonian. Hence one may deduce† the ground-state energy, the mass gap, and the latent heat at the transition point, using the work of Yang and Yang (1966), Johnson *et al* (1973) and Baxter (1973a, b). The conjecture of universality between the statistical mechanics and Hamiltonian field theory formulations is confirmed for this model.

Next, numerical finite-size scaling analyses were performed, both on the original Potts model Hamiltonian and on the equivalent eight-vertex Hamiltonian. Results were obtained for $Q = 4$, 5, 6, 8 and 12. Our conclusions are as follows.

For $Q = 4$, a second-order transition is found at the self-dual point, and the critical exponents are estimated to be $\nu = 0.71 \pm 0.02$, $\alpha/\nu = 0.75 \pm 0.01$ and $\alpha = 0.53 \pm 0.02$. These results are in reasonable agreement with other recent estimates (Ditzian and Kadanoff 1979, Hu 1980, Blöte *et al* 1980), and they satisfy hyperscaling. Unfortunately, they appear incompatible with the universality conjecture above. The most likely explanation of this discrepancy is the presence of logarithmic correction terms of the sort proposed by Nauenberg and Scalapino (1980), and Black and Emery (1981).

For $Q = 5$ and 6, the transition at the self-dual point is impossible to distinguish from a second-order one by our present numerical methods: both the mass gap and the β function appear to vanish there. The reason for this may be seen in the exact solution for the mass gap: it decreases exponentially as $Q \to 4$ from above, and is quite minute for $Q = 5$ and 6. For $Q = 8$ and 12, however, the numerical estimates of the mass gap are definitely greater than zero at the transition point, and in reasonable agreement with the exact solution.

Several methods were tried for estimating the latent heat (i.e. the discontinuity at the transition point in the first derivative of the ground-state energy per site). This proved to be a difficult task to perform with any accuracy, because it is hard to separate the effects of strong curvature *near* the transition point from a discontinuity *at* the transition point. But in the end a particular finite-lattice sequence extrapolation method was tried which had some success. The estimates of the latent heat for $Q = 5$ and 6 were still too high (in these cases the exact solutions are again small), but for $Q = 8$ and 12 they were surprisingly accurate. A similar method could be used to estimate spontaneous magnetisations in finite-lattice analyses.

The finite-size scaling behaviour characteristic of a first-order transition was proposed on physical grounds by Imry (1980). Our results agree with his hypothesis. The finite-lattice specific heats exhibit peaks whose heights increase linearly with lattice size, and whose widths decrease linearly, building up a delta function singularity in the bulk limit.

The layout of the paper is as follows. The Hamiltonian field theory formulation of the Q-state Potts model is reviewed in § 2. The equivalence with an eight-vertex model,

† While revising this paper, we learnt that the ground-state energy and latent heat have also been derived by Kogut, Pearson and Shigemitsu (unpublished).

and exact results at the self-dual point, are derived in § 3. Finite-lattice calculations for the four- and five-state Potts models are presented in § 4, and for the equivalent eight-vertex models in § 5. A summary and conclusions are given in § 6.

2. Formulation

The Hamiltonian field theory version of the Q-state Potts model has been discussed by Sólyom (1980), using the transfer matrix derived by Mittag and Stephen (1971). On a one-dimensional spatial lattice of M sites with a continuous time variable, the lattice Hamiltonian may be written

$$H(\lambda) = -\sum_{i=1}^{M} \sum_{k=1}^{Q-1} (\Omega_i^k + \lambda M_i^k M_{i+1}^{Q-k}), \tag{2.1}$$

where the operators Ω_i and M_i at site i obey the $Z(Q)$ algebra:

$$\Omega_i M_i = \omega^{-1} M_i \Omega_i, \qquad \Omega_i M_i^+ = \omega M_i^+ \Omega_i, \qquad \Omega_i^Q = M_i^Q = 1, \tag{2.2}$$

with

$$\omega \equiv e^{2\pi i/Q}. \tag{2.3}$$

We do not consider any interaction with an external magnetic field. Periodic boundary conditions are applied.

In the strong coupling (high-temperature) region, the operators may be represented on a basis of eigenstates of Ω_i:

$$\Omega_i |w_i\rangle = \omega^{w_i} |w_i\rangle, \qquad w_i = 0, 1, \ldots, Q-1, \tag{2.4}$$

with M_i^+ as ladder operator:

$$M_i^+ |w_i\rangle = |(w_i + 1) \bmod Q\rangle. \tag{2.5}$$

Then $H(\lambda)$ may be reduced to

$$H(\lambda) = \sum_{i=1}^{M} \left((1 - Q\delta_{w_i,0}) - \lambda \sum_{k=1}^{Q-1} M_i^k M_{i+1}^{Q-k} \right). \tag{2.6}$$

In the weak coupling (low-temperature) region, on the other hand, eigenstates of M_i are employed:

$$M_i |m_i\rangle = \omega^{m_i} |m_i\rangle \tag{2.7}$$

and

$$\Omega_i |m_i\rangle = |(m_i + 1) \bmod Q\rangle. \tag{2.8}$$

Then $H(\lambda)$ reduces to

$$H(\lambda) = \sum_{i=1}^{M} \left(\lambda (1 - Q\delta_{m_i, m_{i+1}}) - \sum_{k=1}^{Q-1} \Omega_i^k \right). \tag{2.9}$$

The duality relation for these models is identical to that for the Z_N models (Sólyom 1980, Mittag and Stephen 1971, cf Elitzur *et al* 1979), namely

$$H(\lambda) = \lambda H(1/\lambda). \tag{2.10}$$

It follows that the mass gap $F(\lambda)$ between the ground state and first excited state obeys a

similar relation; so that if the model possesses a single second-order phase transition (i.e. a unique point at which the mass gap vanishes), then it must occur at the self-dual point $\lambda = 1$.

The quantities which will be of interest to us can all be deduced from the lowest two eigenvalues of the Hamiltonian (2.1), E_0 and E_1. They include the mass gap

$$F(\lambda) = E_1(\lambda) - E_0(\lambda), \tag{2.11}$$

the Callan–Symanzik β function (Hamer *et al* 1979)

$$\beta(g)/g = F(\lambda)/[F(\lambda) - 2\lambda\,\partial F/\partial\lambda] \tag{2.12}$$

and the specific heat per site (HB)

$$C(\lambda) = -(\lambda^2/M)\partial^2 E_0(\lambda)/\partial\lambda^2. \tag{2.13}$$

The finite-size scaling and sequence extrapolation techniques which we use to treat these models were summarised in HB. We refer to this paper for details and earlier references.

3. Analytic results

Some exact results are known for the critical behaviour of the two-dimensional Potts model in statistical mechanics (Baxter 1973b, Johnson *et al* 1973). One may derive equivalent results for the corresponding Hamiltonian field theory, as follows.

3.1. Potts model field theory Hamiltonian

For future reference, we first re-derive the field theory Hamiltonian of the Potts model (Sólyom 1980). This may be done by the transfer matrix procedure of Fradkin and Susskind (1978).

The 2D anisotropic Potts model in statistical mechanics has a partition function

$$Z = \sum \exp\left(\sum_{i,j=1}^{M} (K_{\mathrm{H}}\delta_{m(i,j),m(i,j+1)} + K_{\mathrm{V}}\delta_{m(i,j),m(i+1,j)}) \right) \tag{3.1}$$

where i, j label rows and columns of the $M \times M$ lattice, K_{H} and K_{V} are the horizontal and vertical coupling constants, and $m(i, j)$ is the spin on site (i, j), which may take values $0, 1, \ldots, Q-1$. The overall sum runs through all possible spin configurations.

This partition function can be written as the trace of the Mth power of a row-to-row transfer matrix T (Mittag and Stephen 1971), where the matrix T has an element for each possible configuration of spins on two neighbouring rows:

$$T(\sigma_i, \sigma_{i+1}) = \exp\left(\sum_{j=1}^{M} [\tfrac{1}{2}K_{\mathrm{H}}(\delta_{m(i,j),m(i,j+1)} + \delta_{(i+1,j),m(i+1,j+1)}) + K_{\mathrm{V}}\delta_{m(i,j),m(i+1,j)}] \right) \tag{3.2}$$

where σ_i denotes the spin configuration on row i.

Now consider the limit (cf Fradkin and Susskind 1978)

$$\tau \equiv \mathrm{e}^{-K_{\mathrm{V}}} \to 0, \qquad K_{\mathrm{H}} = Q\lambda\ \mathrm{e}^{-K_{\mathrm{V}}}. \tag{3.3}$$

Then the dominant elements of T are the 'diagonal' ones, for which the spin configurations σ_i, σ_{i+1} are identical:

$$T_{\text{diag}} = \exp\Big(MK_{\text{V}} + K_{\text{H}} \sum_{i=1}^{M} \delta_{m(i,j),m(i,j+1)}\Big)$$

$$\to e^{MK_{\text{V}}}\Big(1 + Q\lambda\tau \sum_{i=1}^{M} \delta_{m(i,j),m(i,j+1)}\Big). \tag{3.4}$$

The next most important elements are those for which only one spin is changed in going from row i to row $(i+i)$:

$$T_{1\text{ flip}} \to e^{(M-1)K_{\text{V}}} + O(e^{(M-2)K_{\text{V}}}), \tag{3.5}$$

and all other elements are of higher order in τ. Thus in the limit (3.3) the transfer matrix

$$T \to e^{MK_{\text{V}}}(1 - \tau H) \tag{3.6}$$

where the operator H acting between two rows is

$$H = -\Big(Q\lambda \sum_{j=1}^{M} \delta_{m_j,m_{j+1}} + \sum_{j=1}^{M} \sum_{k=1}^{Q-1} \Omega_j^k\Big). \tag{3.7}$$

Here we have dropped the row index i, and introduced our ladder operator Ω_j of the previous section, which causes a spin flip at column j.

In the above treatment, τ is to be interpreted as a spacing in 'imaginary time' (Fradkin and Susskind 1978), and the limit (3.3) is that in which the time variable becomes continuous. The operator H is then just the equivalent field theory Hamiltonian, up to a constant term—cf the low-temperature representation, equation (2.9).

3.2. An equivalent eight-vertex Hamiltonian

Baxter (1973b) has shown that the two-dimensional Potts model is equivalent to a staggered eight-vertex model, as follows.

The partition function (3.1) can be rewritten

$$Z = \sum \prod_{i,j} (1 + v_{\text{H}}\delta_{m(i,j),m(i,j+1)})(1 + v_{\text{V}}\delta_{m(i,j),m(i+1,j)}) \tag{3.8}$$

where

$$v_{\text{a}} \equiv e^{K_{\text{a}}} - 1. \tag{3.9}$$

This expression can be related to a problem in graph theory (Kasteleyn and Fortuin 1969). Expand the product in (3.8), and for each link on the lattice draw a line if one takes the $v\delta_{m,m'}$ term, no line if one takes unity. The summation over spins can then be performed for each term in the expansion, giving

$$Z = \sum_{G} Q^{C} v_{\text{H}}^{l_{\text{H}}} v_{\text{V}}^{l_{\text{V}}}, \tag{3.10}$$

where the summation is over all graphs G (i.e. all ways of drawing lines on the links of the lattice), C is the number of connected pieces in G (including isolated sites), and l_{H}, l_{V} are the numbers of horizontal and vertical lines in the graph G, respectively.

Temperley and Lieb (1971) have shown that the expression (3.10) is equivalent to

$$Z = Q^{L/2} W(X_{\text{H}}, X_{\text{V}}, Q^{1/2}, Q^{1/2}) \tag{3.11}$$

where W is a 'generalised Whitney polynomial', $L = M^2$ is the number of sites on the lattice, and

$$X_a = v_a / Q^{1/2}. \tag{3.12}$$

They then show that this Whitney polynomial can be related to a staggered eight-vertex model on an auxiliary lattice of $2L$ sites. This model has A and B sublattices alternating as in figure 1(a)). The eight possible vertex types are represented in terms of arrow configurations in figure 1(b)), and in terms of + or − spin variables in figure 1(c)) (the two representations are related by the convention that a positive spin corresponds to a rightgoing arrow, and a negative one to a leftgoing arrow). Our vertices are rotated by 45° relative to the usual convention: this corresponds to the diagonal transfer matrix treatment of Temperley and Lieb.

Using Temperley and Lieb's results, we find that the Potts partition function (3.11) is given by

$$Z = v_H^L Z^* \tag{3.13}$$

where Z^* is the partition function of a staggered eight-vertex model as described above, with vertex weights

$$\begin{aligned} &\text{(A)} \qquad \omega_1, \ldots, \omega_8 = X, X, 1, 1, 0, 0, (X + e^{-\nu}), (X + e^{\nu}), \\ &\text{(B)} \qquad \omega_1', \ldots, \omega_8' = \frac{X}{\lambda}, \frac{X}{\lambda}, 1, 1, 0, 0, \left(\frac{X}{\lambda} + e^{-\nu}\right), \left(\frac{X}{\lambda} + e^{\nu}\right), \end{aligned} \tag{3.14}$$

on the A and B sublattices respectively, where we have introduced new variables

$$X \equiv X_V, \qquad \lambda = X_H X_V, \qquad 2 \cosh \nu = Q^{1/2}. \tag{3.15}$$

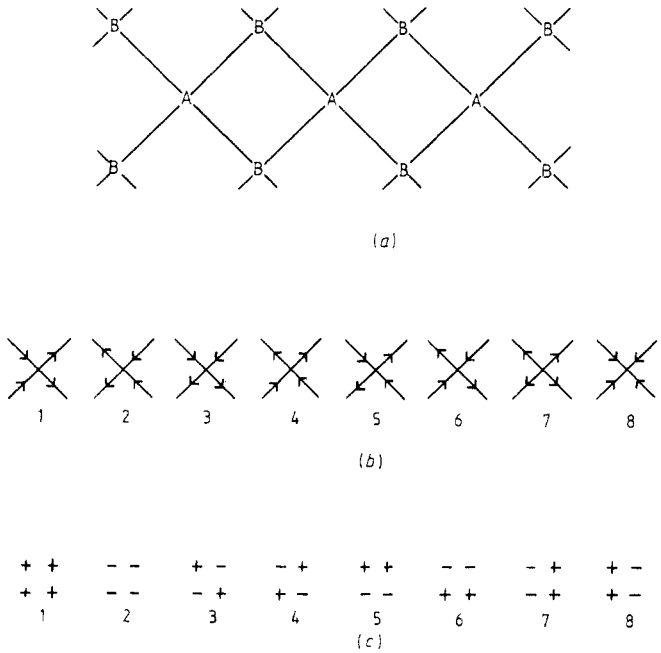

Figure 1. (a) Pattern of A and B vertices on the auxiliary lattice. (b) Arrow representation of the eight possible vertices. (c) Spin representation of the eight possible vertices.

Note that the set of weights (3.14) is only one of several alternative sets, which may be transformed into each other by simultaneously rotating all the vertices in figure 1 by 90°, reversing all arrows on one or other diagonal, etc (see Temperley and Lieb 1971, Baxter 1973b, Fan and Wu 1970).

Now Temperley and Lieb have also shown that the vertices of figure 1 can be expressed in operator form, in terms of Pauli-type operators

$$C = \sigma^X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S = \sigma^Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{3.16}$$

which act between the upper and lower members of a pair of spins in the vertices of figure 1(*c*). Thus we find the operator correspondences

$$\begin{aligned} &I = J_1 + J_2 + J_7 + J_8, && S_1S_2 = J_1 + J_2 - J_7 - J_8, \\ &S_1 = J_1 - J_2 - J_7 + J_8, && S_2 = J_1 - J_2 + J_7 - J_8, \\ &C_1C_2 = J_3 + J_4 + J_5 + J_6, && C_1C_2S_1S_2 = -J_3 - J_4 + J_5 + J_6, \\ &C_1C_2S_1 = -J_3 + J_4 - J_5 + J_6, && C_1C_2S_2 = J_3 - J_4 - J_5 + J_6, \end{aligned} \tag{3.17}$$

where $J_1, \ldots, J_8$ are the vertex operators of figure 1(*c*), S_i and C_i are the Pauli-type operators (3.16), with suffix denoting whether they act on the first or second spin pair, and I is the identity operator.

Then the transfer matrix corresponding to the eight-vertex partition function Z^* can be represented in operator form:

$$\begin{aligned} T^* = \frac{X^{2M}}{\lambda^M} \prod_{A_i} &\left((J_1 + J_2 + J_7 + J_8) + \frac{1}{X}(J_3 + J_4) + \frac{1}{X}(e^{-\nu}J_7 + e^{\nu}J_8) \right) \\ &\times \prod_{B_i} \left((J_1 + J_2 + J_7 + J_8) + \frac{\lambda}{X}(J_3 + J_4) + \frac{\lambda}{X}(e^{-\nu}J_7 + e^{\nu}J_8) \right) \end{aligned} \tag{3.18}$$

where the products run over a row of A vertices and a neighbouring row of B vertices, and at each vertex the operators $J_1, \ldots, J_8$ have been introduced with the weights given in (3.14). Noting that $(J_1 + J_2 + J_7 + J_8)$ is just the identity operator, and taking the Fradkin–Susskind limit $X \to \infty$, one obtains

$$\begin{aligned} T^* \to \left(\frac{X^2}{\lambda}\right)^M \Big(&I + \frac{1}{X} \sum_{A_i} [J_3 + J_4 + \cosh \nu(J_7 + J_8) + \sinh \nu(J_8 - J_7)] \\ &+ \frac{\lambda}{X} \sum_{B_i} [J_3 + J_4 + \cosh(J_7 + J_8) + \sinh(J_8 - J_7)] \Big) \end{aligned} \tag{3.19}$$

$$\equiv (X^2/\lambda)^M (I - \tau H^*), \tag{3.20}$$

where H^* is the field theory Hamiltonian operator for the eight-vertex model. Using the operator correspondences (3.16) and (3.17), this operator can then be rewritten in terms of Pauli matrices:

$$\begin{aligned} H^* = -\frac{Q^{1/2}}{4}(1 + \lambda) \sum_{n=1}^{2M} \Big(&[(\sigma_n^X \sigma_{n+1}^X + \sigma_n^Y \sigma_{n+1}^Y) + \cosh \nu(1 - \sigma_n^Z \sigma_{n+1}^Z)](1 + (-1)^n t) \\ &+ 2t(-1)^n \sinh \nu \sigma_n^Z \Big) \end{aligned} \tag{3.21}$$

where $t=[(1-\lambda)/(1+\lambda)]$, and each site n corresponds to a link along a row of the auxiliary lattice in figure 1(a).

Collecting together multiplicative factors in (3.13) and (3.20), one finds

$$Z=\mathrm{Tr}(T^M) \tag{3.22}$$

where

$$T=v_{\mathrm{H}}^{M}T^{*}\to \mathrm{e}^{MK_{\mathrm{V}}}[1-\tau(M+H^{*})] \tag{3.23}$$

in the Fradkin–Susskind limit (3.3). From (3.6), (3.7), (3.21) and (3.23), one obtains our final result: an eight-vertex model operator equivalent to the Potts model field theory Hamiltonian (2.9) is

$$H'=\left(\frac{1+\lambda}{2}\right)\sum_{n=1}^{2M}\{1-\cosh\nu[1+(-1)^{n}t][(\sigma_n^X\sigma_{n+1}^X+\sigma_n^Y\sigma_{n+1}^Y)$$
$$+\cosh\nu(1-\sigma_n^Z\sigma_{n+1}^Z)]-(-1)^{n}t(\sinh 2\nu)\,\sigma_n^Z\} \tag{3.24}$$

where

$$t=[(1-\lambda)/(1+\lambda)],\qquad \cosh\omega=Q^{1/2}/2. \tag{3.25}$$

We have ignored boundary conditions in the foregoing discussion: these will not affect the thermodynamic limit.

Note also that the equivalence between the Potts model and the staggered eight-vertex model is in fact an equivalence of operator algebras (Temperley and Lieb 1971, Baxter 1981). Hence one expects that not only the ground-state energy, but the whole *set* of allowed energy eigenvalues will be the same for both models; but the degeneracy pattern, or multiplicity of each eigenvalue, will in general be different†.

3.3. Ground-state energy at the critical point

Given the equivalence discussed in § 3.2, it is easy to deduce the properties of the Potts model at the critical point from results in the literature.

At the critical point $\lambda=1$, the eight-vertex Hamiltonian (3.24) reduces to

$$H'(\lambda=1)=\sum_{i=1}^{2M}\left[1-\frac{Q^{1/2}}{2}\left((\sigma_n^X\sigma_{n+1}^X+\sigma_n^Y\sigma_{n+1}^Y)+\frac{Q^{1/2}}{2}(1-\sigma_n^Z\sigma_{n+1}^Z)\right)\right]. \tag{3.26}$$

This is just the well known Heisenberg–Ising Hamiltonian. Its ground-state energy has been calculated by Yang and Yang (1966). The result may be expressed as

$$\lim_{M\to\infty}(E_0(\lambda=1)/M)=2-Q-4Q^{1/2}\int\rho(k)\cos k\,\mathrm{d}k \tag{3.27}$$

where for $0\leqslant Q\leqslant 4$, $\cos\mu\equiv Q^{1/2}/2$, we may replace

$$\cos k=\frac{\cosh\alpha\cos\mu-1}{\cos\mu-\cosh\alpha},\qquad \rho(k)\,\mathrm{d}k=\frac{\mathrm{d}\alpha}{4\mu}\,\mathrm{sech}\left(\frac{\pi\alpha}{2\mu}\right); \tag{3.28a}$$

† I am indebted to Professor R J Baxter for this remark.

while for $Q>4$, $\cosh \nu \equiv Q^{1/2}/2$, we put

$$\cos k = \frac{\cos\alpha \cosh\nu - 1}{\cosh\nu - \cos\alpha}, \qquad \rho(k)\,\mathrm{d}k = \frac{\mathrm{d}\alpha}{4\nu}\operatorname{sech}\left(\frac{\pi\alpha}{2\nu}\right) \tag{3.28b}$$

and the limits on the α integration run from $-\infty$ to $+\infty$.

Substituting (3.28*a*) into (3.27), the expression can be reduced to tabulated integrals for $Q=2, 3, 4$. Thus at $\lambda = 1$,

$$\begin{aligned} \lim_{M\to\infty}(E_0/M) &= -4/\pi && \text{for } Q=2, \\ &= -(\tfrac{4}{3}+2\sqrt{3}(/\pi) && \text{for } Q=3, \\ &= 2-8\ln 2 && \text{for } Q=4. \end{aligned} \tag{3.29}$$

For $Q>4$, using (3.28*b*), one obtains by contour integration

$$\lim_{M\to\infty}\left(\frac{E_0}{M}\right) = 2-Q-Q^{1/2}(Q-4)\sum_{n=1}^{\infty}\frac{(-1)^n}{(\cosh\nu-\cosh(2n+1)\nu)} \tag{3.30}$$

which must be evaluated numerically. Equivalent expressions for the free energy of the 2D isotropic Potts model at the critical point were given by Baxter (1973b).

3.4. Latent heat

Baxter (1973b) has also evaluated the latent heat at the transition point for $Q>4$, in the isotropic Potts model. This may be transcribed to the Hamiltonian field theory formulation, as follows. Transform the eight-vertex model with weights (3.14), thus:

(i) Reverse all the arrows on the upper-left-to-lower-right diagonals in figure 1(*b*): this interchanges vertices $J_1 \leftrightarrow J_4$, $J_2 \leftrightarrow J_3$, $J_5 \leftrightarrow J_7$, $J_6 \leftrightarrow J_8$.

(ii) Next, multiply the weights ω_5 by the quantity

$$\mathrm{e}^{\nu}\left(\frac{(1+X\,\mathrm{e}^{-\nu})[1+(X/\lambda)\,\mathrm{e}^{-\nu}]}{(1+X\,\mathrm{e}^{\nu})[1+(X/\lambda)\,\mathrm{e}^{\nu}]}\right)^{1/4}$$

and the weights ω_6 by its inverse (this operation leaves the partition function unchanged, since the numbers of type 5 and type 6 vertices are equal).

Hence one obtains an equivalent 'ice-type' model, whose weights conform to the pattern of Baxter (1973a), with a 'staggered electric field' E given by

$$\mathrm{e}^{2E} = \left(\frac{(1+X\,\mathrm{e}^{\nu})[1+(X/\lambda)\,\mathrm{e}^{-\nu}]}{(1+X\,\mathrm{e}^{-\nu})[1+(X/\lambda)\,\mathrm{e}^{\nu}]}\right)^{1/2}. \tag{3.31}$$

Thus

$$E \xrightarrow[X\to\infty]{} \frac{(\lambda-1)}{2X}\sinh\nu = \tfrac{1}{2}\tau(\lambda-1)\sinh 2\nu. \tag{3.32}$$

Baxter (1973a) showed that the zero-field spontaneous staggered polarisation in his model is

$$P_0 = \left.\frac{\partial \ln Z}{\partial E}\right|_{E=0} = \prod_{n=1}^{\infty}\tanh^2 n\nu, \tag{3.33}$$

independent of X, or the lattice inhomogeneity. Hence the latent heat we are interested in is

$$\Delta \equiv \lim_{\varepsilon \to 0} \lim_{M \to \infty} \left[\frac{1}{M} \left(\frac{\partial E_0}{\partial \lambda}(\lambda = 1-\varepsilon) - \frac{\partial E_0}{\partial \lambda}(\lambda = 1+\varepsilon) \right) \right] \tag{3.34}$$

$$= \lim_{X \to \infty} \left(\frac{4}{\tau} P_0 \frac{\partial E}{\partial \lambda}\bigg|_{\lambda=1} \right)$$

$$= 2 \sinh 2\nu \prod_{n=1}^{\infty} \tanh^2 n\nu. \tag{3.35}$$

(The definition (3.34) follows from the equivalence between the free energy in statistical mechanics and the ground-state energy in field theory.)

Note that the latent heat vanishes exponentially in the limit $Q \to 4$:

$$\Delta \underset{Q \to 4+}{\sim} 4\pi Q^{1/2} \exp\left(\frac{-\pi^2}{2(Q-4)^{1/2}} \right). \tag{3.36}$$

3.5. Mass gap

The mass gap for the Heisenberg–Ising Hamiltonian (3.26) has been evaluated by Johnson *et al* (1973). Transcribing their result, one finds that for $Q > 4$ there is a mass gap

$$F(\lambda = 1) = (4/\pi) \sinh 2\nu K(1-k^2)^{1/2} \tag{3.37}$$

where K is a complete elliptic integral of the first kind, whose nome is $q = e^{-\nu}$, and whose modulus is k^2. Using standard relations for elliptic integrals, this may be rewritten

$$F(\lambda = 1) = \frac{2 \sinh 2\nu}{(1 + 2\sum_{n=1}^{\infty} q^{n^2})^2} \prod_{n=1}^{\infty} \tanh^4 n\nu \tag{3.38}$$

which is easy to evaluate by numerical means. This quantity also has an essential singularity at $Q = 4$:

$$F(\lambda = 1) \underset{Q \to 4+}{\sim} 8\pi Q^{1/2} \exp\left(\frac{-\pi^2}{(Q-4)^{1/2}} \right). \tag{3.39}$$

Related expressions for the correlation length in the statistical mechanics formulation were discussed by Black and Emery (1981).

4. Finite-lattice results for the four- and five-state Potts model

4.1. Four-state model

The two lowest eigenvalues of the high-temperature Hamiltonian (2.6), together with their relevant derivatives, have been calculated numerically using the methods outlined in HB. At $\lambda = 0$, the ground state has spin $w_i = 0$ at all sites, while the first excited state has a single site with $w_i \neq 0$. The calculations were carried out for chains of up to eight sites, with periodic boundary conditions. The results at the expected critical point, $\lambda = 1$, are listed in table 1.

Table 1. Finite-lattice results for the four-state Potts model as a function of lattice size M. Listed are the critical point estimates λ_M, and values at $\lambda = \lambda_c = 1$ for: the ground-state energy per site E_0/M; the specific heat C_M; the mass gap F_M; the β function β_M/g.

M	λ_M	$-E_0/M$	C_M	F_M	β_M/g
1		6	0	4	1
2	0.749 979 16	4	1.5	1.527 864 04	0.326 237 92
3	0.953 624 66	3.737 0342	2.386 7467	0.965 107 15	0.184 939 15
4	0.982 518 60	3.651 0934	3.130 9808	0.707 687 34	0.124 829 92
5	0.991 081 85	3.612 3571	3.801 5373	0.559 094 26	0.092 199 366
6	0.994 622 98	3.591 5939	4.424 2417	0.462 143 42	0.072 003 040
7	0.996 400 62	3.579 1712	5.012 3690	0.393 841 19	0.058 415 803
8	0.997 413 77	3.571 1482	5.573 8383	0.343 106 44	0.048 728 042

The location of the critical point was computed as the limit of the sequence of values $\{\lambda_M\}$ defined by $R_M(\lambda_M) = 1$, where $R_M(\lambda)$ is the scaled mass gap ratio:

$$R_M(\lambda) = MF_M(\lambda)/(M-1)F_{M-1}(\lambda). \tag{4.1}$$

Extrapolating this sequence by a modified VBS algorithm (see HB), an estimate for the critical point was obtained,

$$\lambda_c = 0.9999 \pm 0.0001, \tag{4.2}$$

which agrees within errors with the expected value. Henceforth we assume $\lambda_c = 1$.

The critical exponent ν was estimated from the finite-lattice sequence of values for the β function (2.12). We form an 'M-shifted' sequence

$$\rho_M(\varepsilon) = (M+\varepsilon)[1-\beta_M(\lambda_c)/\beta_{M-1}(\lambda_c)] \tag{4.3}$$

(where ε is a free parameter), whose limit is

$$\lim_{M\to\infty} \rho_M(\varepsilon) = 1/\nu, \qquad \text{all } \varepsilon, \tag{4.4}$$

by finite-size scaling. Using modified VBS approximants to extrapolate this sequence to the limit, we find the result is stable for $\varepsilon \geqslant 0.6$, leading to an estimate

$$1/\nu = 1.40 \pm 0.03, \qquad \text{or } \nu = 0.71 \pm 0.02. \tag{4.5}$$

The convergence of the sequence is not nearly as good as in the case of the Z_3 or three-state Potts model (HB): this is due, perhaps, to a more complicated singularity structure. The approximants to the sequence $\rho_M(\varepsilon)$ for $\varepsilon = 0.6$ are displayed in table 2.

Table 2. VBS approximants to $1/\nu$ for four-state Potts. The left-hand column lists successive values of the sequence $\rho_M(\varepsilon)$ for $M = 2, 3, \ldots, 8$ and $\varepsilon = 0.6$.

1.751 781			
1.559 217	1.463 094		
1.495 100	1.434 103	1.392 987	
1.463 841	1.420 807	1.395 537	1.398 928
1.445 734	1.413 561	1.396 992	
1.434 148	1.409 203		
1.426 236			

The bulk limit of the β function itself can be estimated by sequence extrapolation (HB) from the finite-lattice form of Romany and Wyld (1980a); the resulting curve is displayed in figure 2. The slope at the critical point should be $-1/2\lambda_c\nu$; thence we obtain $\nu \simeq 0.74$ in agreement with the more accurate result (4.5).

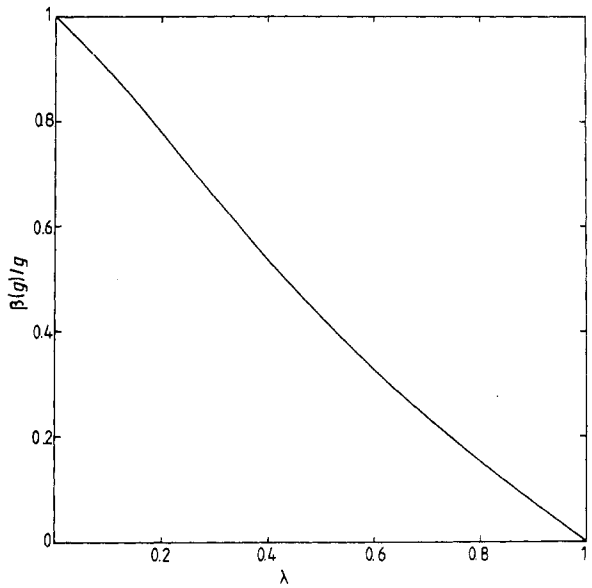

Figure 2. The Callan–Symanzik function $\beta(g)/g$ plotted against λ for the four-state Potts model. The curve was obtained by sequence extrapolation from the Roomany–Wyld finite-lattice estimates. Expected errors are of order the width of the line.

The ratio α/ν can be estimated from the finite-lattice specific heats. The 'M-shifted' sequence

$$\sigma_M(\varepsilon) = (M+\varepsilon)[C_M(\lambda_c)/C_{M-1}(\lambda_c) - 1] \tag{4.6}$$

is expected by finite-size scaling to approach the limit

$$\lim_{M\to\infty} \sigma_M(\varepsilon) = \alpha/\nu, \qquad \text{all } \varepsilon. \tag{4.7}$$

Using modified VBS approximants to extrapolate this sequence, we find the result is stable for $\varepsilon \geq 0$, leading to an estimate

$$\alpha/\nu = 0.75 \pm 0.01 \tag{4.8}$$

or, using (4.5),

$$\alpha = 0.53 \pm 0.02. \tag{4.9}$$

A table of approximants for $\varepsilon = 0$ is displayed in table 3.

4.2. The five-state model

High-temperature Hamiltonian eigenvalues of the five-state model were calculated for chains of up to seven sites. The results at the self-dual point $\lambda = 1$ are displayed in table

Table 3. VBS approximants to α/ν for four-state Potts. The left-hand column lists successive values of the sequence $\sigma_M(\varepsilon)$ for $M = 2, 3, \ldots, 8$ and $\varepsilon = 0.0$.

∞			
1.773 493	1.247 278		
1.247 278	0.981 8416	0.732 2102	
1.070 841	0.895 1915	0.753 3434	0.750 4996
0.982 8198	0.854 0115	0.750 0574	
0.930 5305	0.830 0115		
0.896 1340			

Table 4. Finite-lattice results for the five-state Potts model as a function of lattice size M. Listed are the critical point estimates λ_M, and values at $\lambda = \lambda_c = 1$ for: the ground-state energy per site E_0/M; the specific heat C_M; the mass gap F_M; the β function β_M/g.

M	λ_M	$-E_0/M$	C_M	F_M	β_M/g
1		8	0	5	1
2	0.749 985 93	5.236 0680	2.236 0771	1.848 660 6	0.300 125 50
3	0.952 784 00	4.879 8034	3.731 7375	1.153 350 9	0.162 045 76
4	0.981 433 01	4.764 1094	5.096 8834	0.839 133 64	0.105 453 90
5	0.990 080 47	4.712 1424	6.409 8409	0.659 090 99	0.075 602 337
6	0.993 750 11	4.684 3514	7.697 3521	0.542 245 16	0.057 561 329
7	0.995 645 58	4.667 7520	8.971 9066	0.460 271 04	0.045 671 350

4. From the results of Baxter (1973b), a first-order phase transition is expected to occur at this point.

Carrying through the standard procedure (HB) as for the four-state model, we first attempted to locate a *second*-order critical point by extrapolation of the sequence $\{\lambda_M\}$. The sequence was well converged, and the resulting estimate of the critical point is

$$\lambda_c = 0.9999 \pm 0.0005. \tag{4.10}$$

One is tempted to conclude that $\lambda = 1$ is a *second*-order critical point, i.e. that the mass gap vanishes there. Estimating the critical exponent ν as for the four-state model, one obtains $\nu = 0.65 \pm 0.02$.

But the exact result (3.38) shows that the mass gap is in fact finite at $\lambda = 1$, with an expected value $F = 0.002\,05$. This is so small that it is indistinguishable from zero by current finite-lattice techniques. Indeed, from (4.10) and the apparent index $\nu = 0.65$, one finds that the error estimate in (4.10) is equivalent to an error of ± 0.003 in the mass gap.

The β function was also estimated, as for the four-state model, and the resulting curve is presented in figure 3. It also appears to vanish at a point indistinguishable from $\lambda = 1$.

We next attempt to see whether the transition has a finite latent heat: that is, whether there is a finite discontinuity in the first derivative of the ground-state energy at the critical point.

To start with, the bulk limit of the ground-state energy per site was estimated by sequence extrapolation from the finite-lattice results. The curve so obtained is shown in figure 4. Two points are worthy of note. First, the finite-lattice sequence is especially

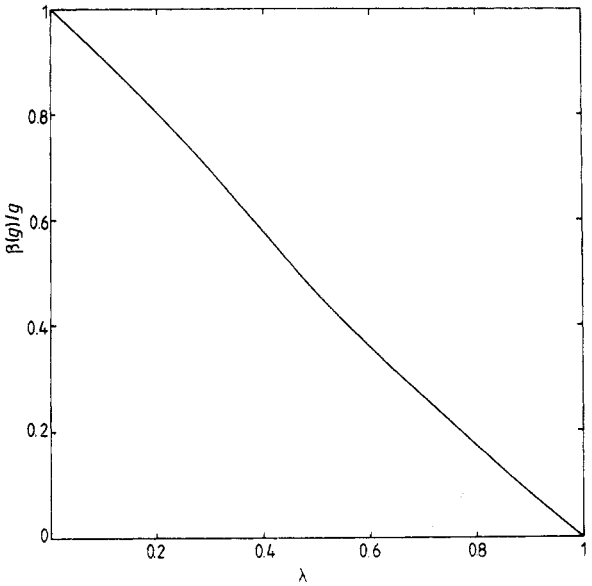

Figure 3. The Callan–Symanzik function $\beta(g)/g$ plotted against λ for the five-state Potts model. The curve was obtained by sequence extrapolation from the Roomany–Wyld finite-lattice estimates. Expected errors are of order the width of the line.

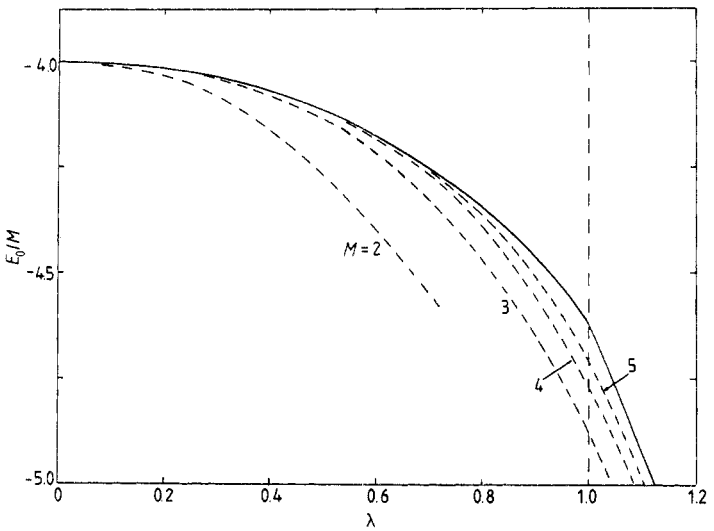

Figure 4. The ground-state energy per site E_0/M plotted against λ for the five-state Potts model. The broken lines are finite-lattice results, labelled by lattice size M; the circled points are estimates of the bulk limit obtained by sequence extrapolation. Expected errors are of order the width of the line.

well behaved at the critical point $\lambda = 1$ (though not in the noman's-land close by on either side), and allows an estimate

$$\lim_{M\to\infty} [E_0(\lambda = 1, M)/M] = -4.622\,55 \pm 0.000\,05, \tag{4.11}$$

in excellent agreement with the exact result (§ 5). Second, there does appear to be a discontinuity in the slope of $E_0(\lambda)/M$ at $\lambda = 1$, which a rough fit by eye gives as

$$\Delta \simeq 1, \tag{4.12}$$

where Δ was defined in (3.34).

Next, the finite-lattice values for $(1/M)\partial E_0/\partial\lambda$ are displayed in figure 5. The 'twisted fan' pattern appears to indicate that a discontinuity is building up as the bulk limit is approached. The finite-lattice sequence again converges very well *at* $\lambda = 1$, but not in the near vicinity on either side; nevertheless, a naive extrapolation (curve a in figure 5) gives

$$\lim_{\varepsilon\to 0}\lim_{M\to\infty}\left(\frac{E_0'(1-\varepsilon)}{M}\right) \simeq -1.5. \tag{4.13}$$

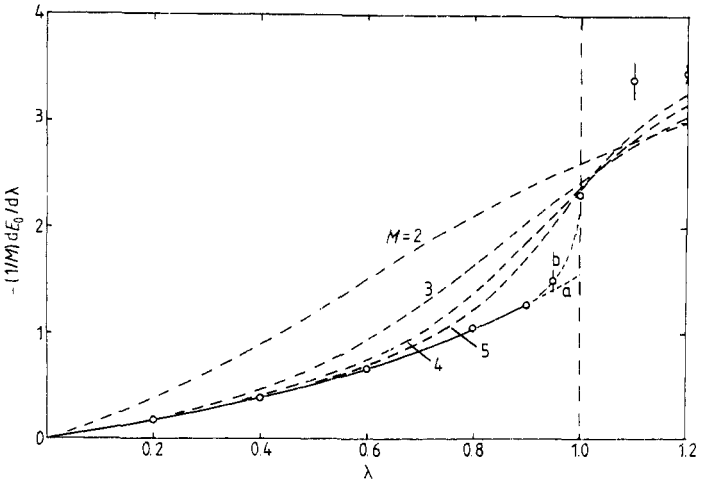

Figure 5. The first derivative $(-E_0'/M)$ plotted against λ for the five-state Potts model. Description as for figure 3. Some rough error bars are shown for the estimates of the bulk limit.

Using the equation

$$\lim_{\varepsilon\to 0}[E_0'(1+\varepsilon)+E_0'(1-\varepsilon)] = E_0(1) \tag{4.14}$$

which follows from the duality equation (2.10), we therefore obtain

$$\Delta \simeq 1.5. \tag{4.15}$$

Finally, the finite-lattice curves for the second derivative $E_0''(\lambda)/M$ are displayed in figure 6. These possess strong peaks near $\lambda = 1$, whose maxima grow linearly with M, and whose widths decrease in an approximately linear fashion. Thus it appears that a delta function is developing in the specific heat as the bulk limit is approached, after the pattern predicted by Imry (1980). We have attempted to estimate its strength by:

(i) fitting a Gaussian or a Lorentzian line shape to each of the finite-lattice curves in the range $0.9 < \lambda < 1.1$;

(ii) finding the integral under each fitted curve;

(iii) extrapolating the sequence so obtained using modified VBS approximants.

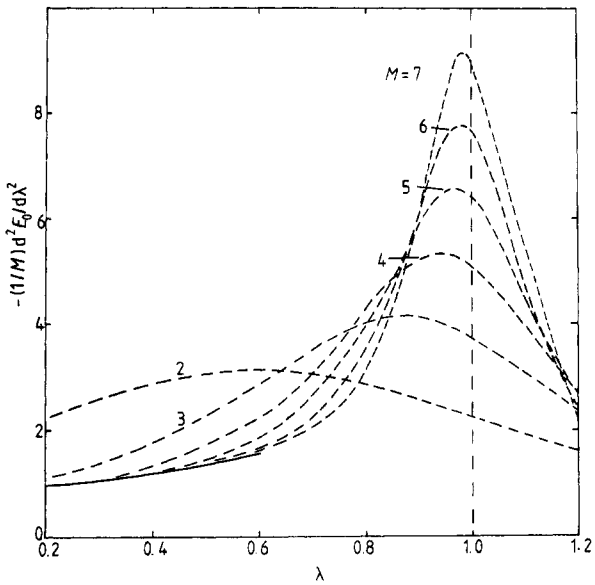

Figure 6. Finite-lattice results for the second derivative $(-E_0''/M)$ plotted against λ for the five-state Potts model.

The result is poor, because the finite-lattice peaks are not well fitted by either a Gaussian or a Lorentzian form, and the sequence is not well converged. But we do obtain a value by this means of

$$\Delta \simeq 1.5. \tag{4.16}$$

Unfortunately, the results (4.12), (4.15) and (4.16) are all too large by an order of magnitude. The exact result, given by (3.35), is $\Delta = 0.173$. It appears that the true first derivative is more like curve b of figure 5, and exhibits strong curvature near $\lambda = 1$ in addition to the latent heat discontinuity. This makes it very difficult to form a reliable estimate of the latent heat.

5. Finite-lattice results for the equivalent eight-vertex model

In order to investigate higher Q values, we have turned to the equivalent eight-vertex model Hamiltonian, equation (3.24), where Q appears merely as a parameter. The two lowest eigenvalues have been calculated for lattices of $2M$ sites, $M = 1, \ldots, 7$, with periodic boundary conditions. The ground state at $\lambda = 0$ contains equal numbers of + and − spins; the first excited state was taken with one extra spin flipped from − to +.

First, the bulk value of the ground-state energy per site was estimated by extrapolation of the finite-lattice sequences, for values of $Q = 4, 5, 6, 8$ and 12. The results were in good agreement† with those of § 4, for $Q = 4$ and 5. The sequences all converged

† Note, that the results for given lattice size M are not exactly identical in the original Potts model (2.6) and in the equivalent eight-vertex model (3.24). This is presumably a boundary effect. The estimated bulk limits do agree, however.

particularly well at the self-dual point $\lambda = 1$: a comparison of our numerical estimates with the exact results is given in table 5. It can be seen that the agreement is excellent.

Table 5. Ground-state energy per site at the critical point $\lambda_c = 1$, for Q-state Potts models with $Q = 4$, 5, 6, 8 and 12. The table compares the numerical values (computed by extrapolation of the finite-lattice sequences) with the exact results derived in § 3.

Q	Numerical result	Analytic result
4	−3.545 18	−3.545 18
5	−4.622 55	−4.622 54
6	−5.679 17	−5.679 22
8	−7.754 2	−7.754 96
12	−11.833	−11.834 70

Next, the mass gap was estimated by similar methods. The results agreed with those for the original Potts model (2.6), within errors, when $Q = 4$ and 5. The estimated mass gaps are plotted against λ in figure 7. For $\lambda \leqslant 0.8$, the sequences converge linearly, and our estimates are expected to be accurate to one per cent or better; but beyond that point, where the mass gaps begin to dip rapidly towards the transition point, the convergence gets worse and our curves become somewhat approximate.

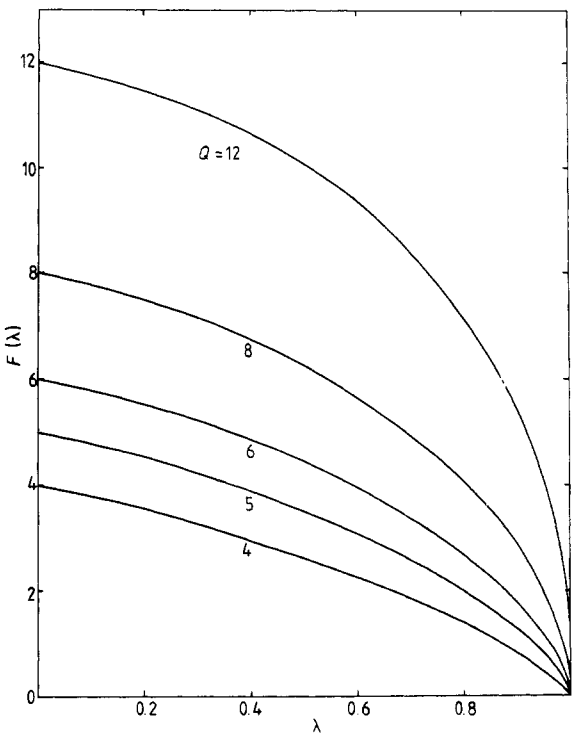

Figure 7. The mass gap $F(\lambda)$ plotted against λ for Q-state Potts models. The curves were obtained by sequence extrapolation of finite-lattice results for the equivalent eight-vertex Hamiltonian. Expected errors are of order the width of the line for $\lambda \leqslant 0.8$, and up to ± 0.2 thereafter.

The mass gap estimates at the transition point; $\lambda = 1$, are compared with the exact analytic result (3.38) in figure 8. It can be seen that the numerical results agree with the analytic ones to about the expected degree of accuracy. But the exponential drop as $Q \to 4$ (equation (3.39)) means that in the cases $Q = 5$ and 6 the mass gap is indistinguishable from zero by our numerical methods: that is, these methods cannot distinguish that the transition is first order rather than second. For the cases $Q = 8$ and $Q = 12$, the result is definitely non-zero, signalling the first-order transition.

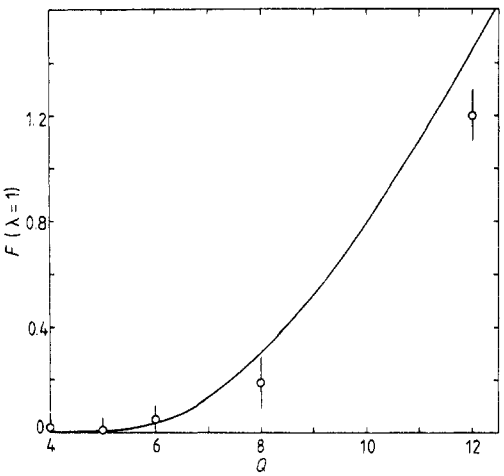

Figure 8. The mass gap at the transition point, $F(\lambda = 1)$, for Q-state Potts models. The full line is the exact analytic result; the circled points are numecal estimates obtained by finite-lattice sequence extrapolation.

Finally, another attempt was made to estimate the latent heat of these transitions. A new method was adopted for this purpose. Recall that our objective is to estimate the quantity $\lim_{\lambda \to 1} \lim_{M \to \infty} [(1/M) \partial E_0(\lambda, M)/\partial \lambda]$ (from which the latent heat can be deduced). Care must be exercised, because the double limit is non-uniform. The procedure we have chosen is to estimate the limit of the sequence

$$\lim_{M \to \infty} \left(\frac{1}{M} \frac{\partial E_0}{\partial \lambda} \bigg|_{\lambda_M = 1 - \varepsilon_0 / M^{\delta}} \right) \tag{5.1}$$

by sequence extrapolation of our finite-lattice results. The sequence of points λ_M must not approach $\lambda = 1$ too *fast*, or we will reach the limits $M \to \infty$, $\lambda \to 1$ in the wrong order, and obtain $\Delta = 0$ (corresponding to the fact that there is no phase transition on a finite lattice). From Imry's result that the width of the region where finite-size effects dominate is $O(1/M)$, this implies a restriction that the index δ in (5.1) must be less than 1. On the other hand, the points λ_M must not approach $\lambda = 1$ too *slowly*, or the sequence (5.1) will itself converge too slowly. Thus we have chosen, arbitrarily, to set the index $\delta = 0.8$.

The limit (5.1) should, in principle, be independent of the parameter ε_0. But if ε_0 is chosen too small, our limited set of results will all lie in the 'finite-size region', and the estimated limit will tend to show $\Delta = 0$, again. For this reason, we restrict $\varepsilon_0 > 0.2$.

Figure 9 shows an example of the estimated limits (5.1), as a function of ε_0, for $Q = 8$. The results from our short sequence are not in fact stable, but vary almost linearly with ε_0; so we have arbitrarily chosen our final estimate as the intercept of this line at $\varepsilon_0 = 0$.

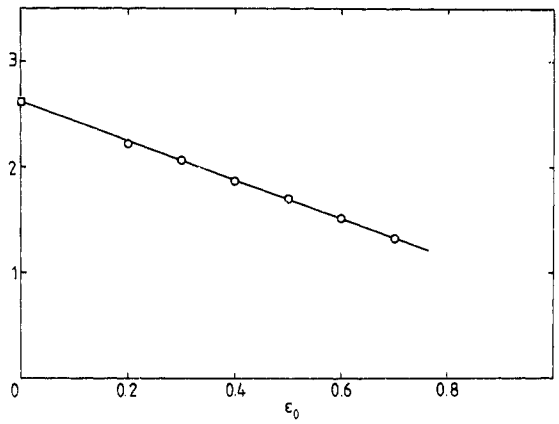

Figure 9. Estimates of the limit (5.1) plotted against the parameter ε_0, with $\delta = 0.8$, for $Q = 8$. The circles are estimates obtained by sequence extrapolation of the finite-lattice results, for various ε_0; the line is a straight-line fit; the square indicates the chosen final estimate.

Having estimated the limit (5.1) in this way, one can deduce the latent heat using equation (4.14). The results are compared with the exact result, equation (3.35), in figure 10. It can be seen that the numerical results are too high for $Q = 5$ and 6, where the latent heat is again trending exponentially to zero, although the estimate for $Q = 5$ is a good deal better than those of § 4. For $Q = 8$ and 12, the numerical results are surprisingly accurate, more so than our rough error bars would lead one to expect: this may be partly fortuitous.

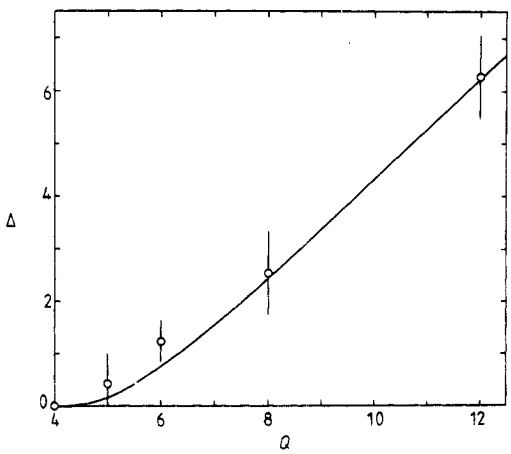

Figure 10. The latent heat Δ plotted against Q, for Q-state Potts models. The full line is the exact analytic result; the circled points are numerical estimates, obtained in the manner outlined in the text.

6. Summary and conclusions

The object of this work was to apply finite-lattice sequence extrapolation techniques (HB) to investigate the behaviour of Q-state Potts models in Hamiltonian field theory, for $Q \geq 4$. We were particularly interested in exploring the application of finite-lattice techniques to a system with a first-order phase transition.

Some aspects of the critical behaviour of these models can be derived exactly. Using the work of Temperley and Lieb (1971), and Baxter (1973b), it is possible to show an equivalence between the Q-state Potts model and a staggered eight-vertex model. Taking the anisotropic limit in the manner of Fradkin and Susskind (1978), one obtains the equivalent eight-vertex field theory Hamiltonian. At the self-dual point $\lambda = 1$, where the phase transition occurs, this Hamiltonian reduces to a simple Heisenberg–Ising form. Its ground-state energy has been derived by Yang and Yang (1966), and the mass gap to the first excited state has been calculated by Johnson *et al* (1973). Using Baxter's (1973a) results, the latent heat in the Hamiltonian field theory was also derived.

Comparing the results found here with those of Baxter (1973b) for the isotropic Potts model, one confirms the universality between the statistical mechanics and the Hamiltonian field theory formulations. In both cases, the transition is first order, with a latent heat which vanishes exponentially (an essential singularity) as $Q \to 4$. From the Fradkin–Susskind (1978) limiting procedure, it is obvious that this universality must hold for any model, in fact, whose critical behaviour is universal with respect to anisotropic couplings.

The later sections of the paper concerned the numerical finite-lattice work. In general, the finite-lattice sequences did not converge as well as for the Z_3 or three-state Potts model treated by HB. Nevertheless, we believe our results to be somewhat more reliable and accurate than previous analyses.

The findings for the models considered were the following.

6.1. Four-state Potts model

A second-order critical point was found to lie at the self-dual point $\lambda = 1$ (as expected), within errors $\pm 0.01\%$. The critical exponents were estimated to be

$$\begin{aligned} \nu &= 0.71 \pm 0.02, \\ \alpha/\nu &= 0.75 \pm 0.01, \end{aligned} \tag{6.1}$$

and hence

$$\alpha = 0.53 \pm 0.02.$$

The sequences for these exponents were a little unstable, which may indicate the presence of more complicated singularities of some sort.

These results agree quite well with previous finite-lattice estimates: Roomany and Wyld (1980b) obtained a value $\nu \simeq 0.76$, and Blöte *et al* (1980) found $y_T \equiv 1/\nu = 1.37$ (reading off their figure 1). They also agree with the latest series estimate, that of Ditzian and Kadanoff (1979), who found $\alpha = 0.50 \pm 0.05$. Finally, they satisfy the hyperscaling relations within errors: e.g. for $\alpha/\nu = \frac{3}{4}$, hyperscaling would predict $\nu = \frac{8}{11} = 0.727$, $\alpha = \frac{6}{11} = 0.545$.

Our results apear inconsistent, however, with the universality conjecture $\alpha = \nu = \frac{2}{3}$, $\alpha/\nu = 1$, $y_T = \frac{3}{2}$ (Enting 1975, Kadanoff 1977, Domany and Riedel 1978, den Nijs

1979). The result for α/ν, in particular, appears incompatible with the conjecture. Now the presence of confluent power-law singularities should not affect our method (Barber and Hamer 1980), except to slow the rate of convergence. But the method is vulnerable to logarithmic corrections to scaling, of the sort suggested for this model by Nauenberg and Scalapino (1980) and Black and Emery (1981). If one multiplies the terms of the sequence $\sigma_M(\varepsilon)$ by $[1+\ln(M)]$, for instance, then the apparent limit of the sequence changes to 0.92. So a term of this type may explain the apparent discrepancy with universality.

6.2. Five-state Potts model

This model was also treated separately, using the original Potts Hamiltonian.

By all the numerical tests, it was impossible to distinguish the transition in this model from a second-order one. Both the mass gap† and the β function appeared to vanish at the self-dual point $\lambda = 1$, within errors. The reason for this can be seen from the exact solution, equation (3.38), which contains an essential singularity at $Q = 4$. The mass gap at $Q = 5$ is thus exponentially small ($F(\lambda = 1) = 0.002$), and impossible to distinguish from zero by our numerical methods. Similar conclusions have been reached by other authors: for instance, the high-temperature series analysis of Kim and Joseph (1975), who found evidence that the susceptibility diverges at or near the transition point; and the finite-size scaling analysis of Roomany and Wyld (1980b), who found a second-order transition there.

A study of the ground-state energy revealed evidence for a discontinuity in its slope at $\lambda = 1$, i.e. a first-order phase transition. Several crude methods were tried in this section for estimating the latent heat. They all gave $\Delta \simeq 1-1.5$, an order of magnitude larger than the exact value $\Delta = 0.17$. There appears to be some strong curvature near $\lambda = 1$ in the quantity E_0'/M, in addition to the discontinuity, and it is very difficult to separate the two effects.

It is interesting to note the characteristic features of a first-order phase transition, as observed in a finite-lattice calculation of the present type. There is no hysteresis phenomenon, such as was observed in the Monte Carlo calculations of Creutz *et al* (1979), because the present method always gives the exact (or 'equilibrium') ground state. Instead, the first-order transition is signalled by finite-lattice peaks in E_0''/M whose heights increase (and whose widths decrease) linearly with lattice size M. Physical arguments which lead to this conclusion have been given by Imry (1980). In the bulk limit these peaks will develop into a delta function singularity.

6.3. General Q-state Potts models

In § 5, a finite-lattice analysis of the equivalent eight-vertex Hamiltonian was carried out, for $Q = 4$, 5, 6, 8 and 12. The results for $Q = 4$ and 5 agreed within errors with those above. Numerical estimates were made by sequence extrapolation of finite-lattice results for the ground-state energy, the mass gap and the latent heat. The results

† It is worth emphasising that the first excited state involved here is a local excitation containing an extra 'flipped' spin, which controls the correlation length in the model, and lies in a disjoint sector of states from the ground state. A first-order phase transition involves the crossing of two 'vacuum' eigenvalues, and the 'mass gap' between these two states will *automatically* vanish at the transition point. We have not looked for this 'metastable vacuum' state.

at the transition point, $\lambda = 1$, were displayed as functions of Q in table 5 and figures 8 and 10.

The estimated ground-state energies agreed with the exact results to an excellent accuracy, of order 1 part in 10^5. The mass gaps could not be estimated so accurately, and for $Q = 5$ and $Q = 6$ they were indistinguishable from zero, within errors: that is, these cases could not be distinguished from second-order transitions. This is because of the strong essential singularity in the mass gap at $Q = 4$, which implies exponentially small values nearby. For $Q = 8$ and $Q = 12$, the numerical estimates were definitely non-zero, and were in approximate agreement with the exact results.

Finally, a new method was tried for estimating the latent heat of these transitions, which had some success. The non-uniform double limit,

$$\lim_{\lambda \to 1} \lim_{M \to \infty} [(1/M) \partial E_0(\lambda, M)/\partial \lambda],$$

was estimated as the limit of a sequence of finite-lattice values taken at points

$$\lambda_M = 1 - \varepsilon_0 / M^{\delta}, \tag{6.2}$$

with δ restricted to be less than 1 (the actual value chosen was 0.8), and ε_0 arbitrary. The sequence (6.2) approaches $\lambda = 1$ more slowly than the region of finite-size rounding does, which according to Imry (1980) goes like $O(1/M)$; thus the sequence is expected to give us the correct limit. In practice, the estimated limit was found to vary somewhat with ε_0, due to the restricted length of the sequence available, and an extrapolation to $\varepsilon_0 = 0$ was made to achieve the final estimate. The results were still too high for $Q = 5$ and 6, where the latent heat is small, but were surprisingly accurate for $Q = 8$ and 12. A similar method could be used in calculating spontaneous magnetisation values from a finite-lattice approach.

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