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Finite-lattice extrapolations for Z_3 and Z_5 models

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Abstract. A method is presented to accelerate the convergence of finite-lattice sequences to their bulk limit. The calculation of highly accurate estimates of the critical parameters of the bulk system is then possible. Applied to the Hamiltonian version of the Z_3 model (three-state Potts model) in $(1+1)$ dimensions, these techniques yield estimates for the exponents $\gamma = 1.444 \pm 0.001$, $\nu = 0.8333 \pm 0.0003$ and $\alpha = 0.33 \pm 0.01$. For the Z_5 model, the presence of a Kosterlitz–Thouless transition is confirmed.

1. Introduction

The finite-size scaling theory of Fisher and Barber (1972) has been formulated in the context of Hamiltonian lattice field theory† by the present authors (Hamer and Barber 1980). This approach involves the calculation of the eigenvalues of the lattice Hamiltonian on a sequence of finite lattices of increasing size. From the way in which these eigenvalues (and other derived quantities of physical interest) scale with the size of the lattice, one may infer the critical behaviour (if any) of the bulk, infinite system. This scheme has been successfully tested on various Hamiltonians in $(1+1)$ dimensions (Hamer and Barber 1981a, b). Other applications and some significant theoretical extensions have also been made by an Urbana group (Roomany *et al* 1980, Roomany and Wyld 1980, 1981).

The finite-lattice sequences which arise in these calculations generally display a smooth and regular convergence towards their bulk limit. The purpose of the present work is to show that this convergence can be substantially *accelerated* by sequence transformation methods. As a result, very accurate estimates for the bulk critical parameters can be obtained.

The particular sequence transformations we employ are due to Vanden Broeck and Schwartz (1979). These authors presented a family of sequence transformations depending on an arbitrary real parameter α, which includes the Padé table ($\alpha = 1$) and the iterated Aitken–Shanks table ($\alpha = 0$) as special cases. By judicious choice of the parameter α, Vanden Broeck and Schwartz were able successfully to accelerate the convergence of a wide variety of sequences. Elsewhere (Barber and Hamer 1981), we have shown analytically that by choosing $\alpha = -1$, the estimate of the limit of a sequence converging as $O(n^{-\lambda})$, as $n \to \infty$, can be markedly improved. Since this type of behaviour is expected in finite-lattice sequences near a critical point, this particular

† For an introduction to Hamiltonian lattice field theories of spin and gauge systems, see Kogut (1979).

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sequence transformation should significantly increase the accuracy of the lattice extrapolation procedure.

We find that this hope is fulfilled. Specifically, we apply the technique to the Z_3 and Z_5 spin models in $(1+1)$ dimensions. For the Z_3 model, which is equivalent to the three-state Potts model, we obtain the estimates of the critical exponents $\nu = 0.8333 \pm 0.0003$, $\gamma = 1.444 \pm 0.001$ and $\alpha = 0.33 \pm 0.01$. (The specific heat exponent α mentioned here should not be confused with the Vanden Broeck and Schwartz parameter introduced earlier.) These results are in excellent agreement with the universality hypothesis (Alexander 1975) that the three-state Potts model should have the same exponents as the 'hard hexagon' model of Baxter (1980), namely $\nu = \frac{5}{6}$, $\gamma = \frac{13}{9}$ and $\alpha = \frac{1}{3}$.

For the Z_5 model, our results agree qualitatively with those of the perturbation calculation of Elitzur *et al* (1979). We find a three-phase structure with an exponential Kosterlitz–Thouless type transition at the dual critical points delimiting the central massless phase. For the strong-coupling critical point we find $\lambda_c = 0.990 \pm 0.005$, and for the exponential index we find $\sigma = 0.6 \pm 0.1$, consistent with the standard Kosterlitz–Thouless value of $\sigma = 0.5$ (Kosterlitz 1974).

The layout of the paper is as follows. In § 2, we discuss the methods employed. First we summarise the essential formulae involved in (a) Hamiltonain lattice field theory for Z_p models and (b) finite-size scaling. In § 2.3 the sequence extrapolation techniques are presented. Section 3 contains the results of the calculations for the Z_3 model and § 4 those for the Z_5 model. Section 5 consists of an overall summary and conclusion. Lastly, there is an Appendix on numerical methods.

2. Methods

2.1. Hamiltonian field theory for Z_p models

The Hamiltonian field theory version of the Z_p models has been given by Elitzur *et al* (1979, henceforth referred to as EPS). On a one-dimensional spatial lattice of M sites with a continuous time variable, the lattice Hamiltonian in the strong-coupling regime is

$$H(\lambda, h) = -\sum_{i=1}^{M} [\cos(2\pi L_i/p) + \tfrac{1}{2}\lambda(R_i^+ R_{i-1}^- + R_i^- R_{i-1}^+) - \tfrac{1}{2}h(R_i^+ + R_i^-)], \tag{2.1}$$

where we apply periodic boundary conditions so that $R_{M+i}^{\pm} = R_i^{\pm}$. The operators L_i have as their spectrum Z_p, the integers modulo p, and $R_i^{\pm}$ are raising and lowering operators for the 'spin' L_i. The parameter $\lambda = 2/g^2$ (where g is the conventional field theory coupling) plays the role of temperature. Finally, h is an external symmetry breaking 'magnetic' field which preferentially selects one of the p equivalent states of spin L_i. The cases $p = 2$ and $p = 3$ are equivalent to the Ising and three-state Potts models respectively.

The Z_p models are self-dual; subject to appropriate boundary conditions, the Hamiltonian (2.1) satisfies the relation (EPS)

$$H(\lambda) = \lambda H(1/\lambda). \tag{2.2}$$

Thus the mass gap $F(\lambda)$ between the ground state and the first excited state obeys a similar relation,

$$F(\lambda) = \lambda F(1/\lambda). \tag{2.3}$$

It then follows that if there is a single second-order phase transition in such a model (i.e. a unique point at which the mass gap vanishes), it must occur at the self-dual point $\lambda = 1$.

The correspondences between Hamiltonian field theory and statistical mechanics are by now well established (see e.g. Kogut 1979, Hamer *et al* 1979, Hamer and Kogut 1979, Hamer and Barber 1981a, b). All quantities of interest to us can be deduced from the lowest two eigenvalues of the Hamiltonian (2.1), E_0 and E_1. In particular, the mass gap, or inverse correlation length, is

$$F(\lambda, h) = E_1(\lambda, h) - E_0(\lambda, h), \tag{2.4}$$

while the Callan–Symanzik β function is given by (Hamer *et al* 1979)

$$\beta(g)/g = F(\lambda, 0)/[F(\lambda, 0) - 2\,\partial F(\lambda, 0)/\partial \ln \lambda\,]. \tag{2.5}$$

We now turn to thermodynamic quantities. The free energy corresponds to the ground state energy, $E_0(\lambda, h)$ with λ playing the role of temperature. Thus the 'specific heat' is

$$C(\lambda) = -\frac{\lambda^2}{M}\frac{\partial^2}{\partial \lambda^2} E_0(\lambda, 0), \tag{2.6}$$

while the 'zero-field susceptibility' is

$$\chi(\lambda) = -\frac{1}{M}\frac{\partial^2}{\partial h^2} E_0(\lambda, h)|_{h=0}. \tag{2.7}$$

All aspects of critical behaviour of interest in statistical mechanics can consequently be investigated from the Hamiltonian field-theoretic formulation. We shall explore the critical behaviour of Z_3 and Z_5 using finite-size scaling.

2.2. Finite-size scaling methods

We have previously discussed (Hamer and Barber 1980, 1981a, b) the application of finite-size scaling techniques to Hamiltonian field theory. Let us briefly summarise the essential points.

The basic procedure is to calculate the eigenvalues of the Hamiltonian on a sequence of lattices of finite size and to derive from them the quantities given in equations (2.4)–(2.7). The asymptotic behaviour of these sequences for M large but finite is prescribed by finite-size scaling (Fisher and Barber 1972) in terms of the critical parameters of the bulk system.

Two regimes of coupling are of interest to us. For $\lambda < \lambda_c$, the critical coupling of the infinite system, the finite-lattice estimates A_M of any quantity A are expected to approach† the bulk limit A_∞ as

$$A_M - A_\infty = \mathrm{O}\{\exp[-\text{constant}\, M F_\infty(\lambda)]\} \tag{2.8}$$

where $F_\infty(\lambda)$ is the mass gap of the infinite system. As $\lambda \to \lambda_c$, this exponential convergence breaks down.

To determine the behaviour of finite-size estimates *at* λ_c, we make the crucial assumption (Fisher and Barber 1972) that at λ_c the correlation length is proportional to the linear dimension of the finite lattice (the maximum it can be). Consequently the

† This is true in the case of periodic boundary conditions of interest here. Other boundary conditions give rise to algebraic corrections in M^{-1}.

mass gap varies as

$$F_M(\lambda_c) \sim \text{constant}/M \qquad \text{as } M \to \infty. \tag{2.9}$$

A series of estimates $\{\lambda_M\}$ of the position of the critical point can thus be calculated by forming (Hamer and Barber 1980) the 'scaled mass gap ratio' for successive lattice sizes,

$$R_M(\lambda) \equiv MF_M(\lambda)/(M-1)F_{M-1}(\lambda), \tag{2.10}$$

and defining λ_M by the solution of

$$R_M(\lambda) = 1. \tag{2.11}$$

Other quantities are assumed to scale in proportion to the mass gap: more specifically, if $\Psi(\lambda)$ is some quantity which diverges in the bulk system as

$$\Psi(\lambda) \sim A|\lambda_c - \lambda|^{-\psi}, \qquad \lambda \to \lambda_c, \tag{2.12}$$

then on a lattice of M sites, $\Psi_M(\lambda_c)$ should scale as

$$\Psi_M(\lambda_c) \sim \text{constant}\, M^{\psi/\nu}, \tag{2.13}$$

where ν is the exponent of the bulk correlation length. Hence one can estimate the ratio ψ/ν from the sequence

$$M[\Psi_M(\lambda_c) - \Psi_{M-1}(\lambda_c)]/\Psi_{M-1}(\lambda_c) \to \psi/\nu \qquad \text{as } M \to \infty. \tag{2.14}$$

The corrections† to the limit are expected to be algebraic in M^{-1}. The exponent ν itself follows, since the β function is expected to vanish linearly at λ_c, and therefore the finite-lattice estimates $\beta_M(\lambda_c) \sim M^{-1/\nu}$.

Roomany and Wyld (1980) have recently shown how finite-size scaling can be regarded as a renormalisation-group technique (see also Suzuki 1977, Nightingale 1977, Sneddon and Stinchcombe 1979). This treatment leads to an alternative way of estimating the β function via the approximants

$$\frac{\beta_M^{\mathrm{RW}}(g)}{g} = [\ln R_M(\lambda)]\left[\left(1 - \lambda\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln[F_M(\lambda)F_{M-1}(\lambda)]\right)\ln\left(\frac{M}{M-1}\right)\right]^{-1}, \tag{2.15}$$

which converge remarkably quickly even for quite small values of M. The scaling formula (2.13) does not apply to β_M^{RW}, since the lattice-size dependence has already been 'scaled out' by the use of results from two consecutive M values.

The numerical methods which may be used to calculate the finite-lattice eigenvalues have been presented elsewhere (Hamer and Barber 1981b, Roomany *et al* 1980). Some further comments are made in the Appendix.

2.3. Sequence extrapolation techniques

The finite-size scaling techniques summarised above seem to work quite well in practice (Hamer and Barber 1981a, b, Roomany *et al* 1980, Roomany and Wyld 1980, 1981). For example, for the Hamiltonian version of the two-dimensional Ising model, the results for chains of $M \leqslant 10$ sites give estimates of the critical point accurate to 0.1%

† For the Ising model, one can show analytically (Hamer and Barber 1981a) that the corrections are at least $O(M^{-2})$; more generally, one expects them to involve the Wegner (1972) correction-to-scaling exponent and hence be stronger.

and of the critical exponents to 0.5% (Hamer and Barber 1981a). For other models the accuracy is, however, rather less.

Our object now is to explore the possibility of accelerating the convergence of the finite-lattice sequences and thereby to improve the estimates of the bulk critical parameters. Techniques of this sort, such as Neville tables, are already commonly used in conjunction with series analyses in statistical mechanics (see e.g. Gaunt and Guttmann 1974, Hunter and Baker 1973).

The particular sequence transformations we employ are due originally to Vanden Broeck and Schwartz (1979). Given a sequence of values A_M which converge to some limiting value $A_\infty = \lim_{M\to\infty} A_M$, one forms a table of approximants to A_∞ denoted by $[M, L]$, where

$$[M, 0] = A_M \tag{2.16}$$

and the $(L+1)$th column of approximants is generated from the Lth and $(L-1)$th columns via the formula

$$\frac{1}{[M, L+1]-[M, L]} + \frac{\alpha_L}{[M, L-1]-[M, L]} = \frac{1}{[M+1, L]-[M, L]} + \frac{1}{[M-1, L]-[M, L]}, \tag{2.17}$$

with the auxiliary condition $[M, -1] = \infty$ imposed. The set of real parameters $\{\alpha_L\}$ is arbitrary. We shall refer to these approximants as 'VBS approximants'.

This general family of transformations includes some well known special cases. For $\alpha_L \equiv 1$, for all L, Wynn's ε algorithm for generating the Padé table (Wynn 1966) is recovered, while with $\alpha_L \equiv 0$, for all L, the transformation is equivalent to an iterated Aitken–Shanks table (Shanks 1955). The hope is that each column of the table will be more rapidly convergent than its predecessor.

There is, however, little theory behind the use of the transformations or in the selection of an 'optimal' value for the α's. Our exploitation of the transforms is based on two observations. Firstly, if the original sequence elements are *exactly* in geometric progression,

$$A_M = [M, 0] = B + cq^M, \tag{2.18}$$

then one application of the transformation (2.17), with effectively $\alpha_0 = 0$, eliminates the 'transient' cq^M and gives the correct limit B. Thus sequences converging as in (2.8) should be considerably accelerated† by iterating (2.17) with $\alpha_L \equiv 0$.

We have tested this possibility on the Ising (Z_2) model for which the bulk limit is known (Pfeuty 1970). Table 1 shows a typical extrapolation for the mass gap at $\lambda = 0.6$ ($\lambda_c = 1$). The first column lists a sequence of finite-lattice estimates taken from the exact results of Hamer and Barber (1981a) for $M \leqslant 10$. Successive columns give the VBS approximants using $\alpha_L = 0$ for all L. While the original finite-lattice estimates have evidently converged to $\frac{1}{4}$% of the exact limit of 0.8, use of the approximants improves this convergence by another four orders of magnitude.

The second relevant observation regarding the transformations (2.17) concerns the acceleration of sequences converging as

$$A_M \sim A_\infty + bM^{-\lambda_1} + b_2M^{-\lambda_2} + \cdots, \qquad M \to \infty, \tag{2.19}$$

† This is actually an example of the Aitken–Delves δ^2 algorithm of numerical analysis applicable to linear convergence (see e.g. Ralston 1965).

Table 1. Table of VBS approximants ($\alpha = 0$) to the Ising model mass gap for $\lambda = 0.6$. The left-hand column consists of successive finite-lattice results, for $M = 2$ to 10.

1.132 3818				
0.943 5596	0.823 5581			
0.870 1880	0.807 3633	0.800 5777		
0.836 3431	0.802 5814	0.800 1872	0.800 0100	
0.819 4415	0.800 9860	0.800 0653	0.800 0020	0.800 0005
0.810 6192	0.800 4022	0.800 0236	0.800 0007	
0.805 8850	0.800 1725	0.800 0089		
0.803 2962	0.800 0770			
0.801 8613				

where $\lambda_1 < \lambda_2$. Elsewhere (Barber and Hamer 1981) we have shown analytically that if $A_M = [M, 0]$ satisfies (2.19), then

$$[M, 2] = A_\infty + O(M^{-\lambda'}) \tag{2.20}$$

provided $\alpha_1 = -1$. The value of λ' is the minimum of λ_2 and $\lambda_1 + 2$. Again this result can be iterated, the appropriate values of α_L being

$$\alpha_L = -[1-(-)^L]/2, \qquad L = 0, 1, 2, \cdots. \tag{2.21}$$

This is the transformation we use in the subsequent analysis of finite-lattice sequences in the vicinity of the bulk critical point.

Since the apparent convergence of the VBS tables can sometimes be misleading, we have found it useful to 'M-shift' our sequences: that is, we add another parameter ε by replacing the multiplying factor M in (2.14) by $(M + \varepsilon)$. Shifts of this form are common in the ratio analysis of series coefficients (see e.g. Gaunt and Guttmann 1974). The exact limit of the sequence (2.14) is unaffected by this change, which, however, has the effect of decreasing the significance of corrections which are integral powers of M^{-1}. In addition, by looking at the stability of the table of VBS approximants with respect to changes in ε, one may both select the 'best estimate' for the limit and obtain some idea of its accuracy.

3. Results for Z_3 model

The Z_3 model, as noted earlier, is equivalent to the three-state Potts model for which a conventional critical point is expected. A finite-size analysis† of the mass gap has been reported previously by Roomany *et al* (1980). However, as we shall see, the accuracy of this calculation can be considerably improved by the use of a table of VBS approximants.

The two lowest eigenvalues of the Hamiltonian (2.1), together with their relevant derivatives, have been computed using the methods summarised in the Appendix. These calculations were carried out for chains of up to ten sites with periodic boundary conditions. The results for various quantities of interest are listed in table 2. These data are correct to the last figure quoted, and for the mass gap probably to 10^{-12}.

† Finite-size scaling has also been used, by Nightingale and Blöte (1980), to investigate the conventionally formulated three-state Potts model.

Table 2. Finite-lattice results for the Z_3 model as a function of lattice size M. Listed are the critical point estimates λ_M and values at $\lambda = \lambda_c = 1$ of the mass gap F_M, the β function β_M/g; the specific heat C_M and the susceptibility χ_M.

M	λ_M	F_M	β_M/g	C_M	χ_M
1			1.000 000 000	0	0.666 658
2	0.752 806 51	0.594 592 199	0.361 661 031	0.433 0124	2.821 367
3	0.954 284 77	0.380 157 223	0.217 322 900	0.652 6328	5.943 208
4	0.983 534 03	0.280 646 979	0.153 075 335	0.819 0950	9.936 795
5	0.992 038 47	0.222 732 323	0.116 976 574	0.957 9403	14.739 091
6	0.995 454 11	0.184 734 369	0.093 994 260	1.079 0415	20.304 015
7	0.997 112 27	0.157 853 417	0.078 156 144	1.187 4918	26.595 732
8	0.998 024 70	0.137 820 880	0.066 623 193	1.286 3330	33.585 213
9	0.998 573 60	0.122 309 965	0.057 876 606	1.377 5694	41.247 03
10	0.998 926 56	0.109 942 479	0.051 032 229	1.462 5929	

3.1. Critical point

We consider first the sequence for the critical coupling. This sequence consists of the values λ_M such that $R_M(\lambda_M) = 1$, where $R_M(\lambda)$ is the scaled mass-gap ratio defined by (2.10). To determine λ_M, the equation $R_M(\lambda) = 1$ was solved by extrapolation from a cluster of five points about $\lambda = 1$ using finite-difference methods.

The sequence of values of λ_M listed in table 2 already suggests $\lambda_c \simeq 1$. The VBS table with α_L specified by (2.21) converges extremely fast and yields the estimate

$$\lambda_c = 1.000\,00 \pm 0.000\,05. \tag{3.1}$$

This result confirms with high accuracy the EPS conclusion that the Z_3 model has two phases, separated by the self-dual point $\lambda = \lambda_c = 1$. For the remainder of our Z_3 calculations, we shall assume that λ_c is exactly unity.

3.2. β function

Turning now to the critical exponents, we estimate first $1/\nu$ using the finite-lattice estimates of the β function (2.5) together with (2.13) and (2.14). As described in § 2.3, the initial estimates are 'M-shifted'. That is, we form the sequence

$$\rho_M(\varepsilon) = (M + \varepsilon)[\beta_{M-1}(\lambda_c) - \beta_M(\lambda_c)]/\beta_{M-1}(\lambda_c), \tag{3.2}$$

where ε is a free parameter. In view of (2.13),

$$\lim_{M\to\infty} \rho_M(\varepsilon) = 1/\nu \tag{3.3}$$

for all ε.

Table 3 presents the tables of VBS approximants to (3.2) for $\varepsilon = 0$ and $\varepsilon = 0.7$; both are reasonably convergent. To distinguish between them, we refer to figure 1, which is a plot of the last iterate against ε. The significant feature is the relative insensitivity to ε over the range $\varepsilon \geqslant 0.4$. Thus we take the table of VBS approximants for $\varepsilon = 0.5$ as our 'best' extrapolation and conclude that

$$1/\nu = 1.2000 \pm 0.0005. \tag{3.4}$$

Table 3. VBS approximants to $1/\nu$ for Z_3 model. The left-hand column lists successive values of the sequence $\rho_n(\varepsilon)$ defined by (3.2) for $M = 2, 3, \ldots, 10$ and the indicated value of the M-shift ε.

(*a*) $\varepsilon = 0.0$				
1.276 678				
1.197 294	1.179 153			
1.182 527	1.178 094	1.178 477		
1.117 912	1.178 787	1.178 960	1.178 924	
1.178 816	1.179 026	1.178 921	1.178 963	1.178 965
1.179 506	1.177 267	1.178 323	1.178 965	
1.180 504	1.162 603	1.169 538		
1.181 550	1.212 278			
1.182 581				
(*b*) $\varepsilon = 0.7$				
1.723 515				
1.476 662	1.341 853			
1.389 470	1.295 290	1.200 474		
1.344 194	1.271 839	1.200 392	1.200 593	
1.316 345	1.257 646	1.200 252	1.199 889	1.200 015
1.297 457	1.248 115	1.200 151	1.200 156	
1.283 798	1.241 267	1.200 156		
1.273 459	1.236 109			
1.265 362				

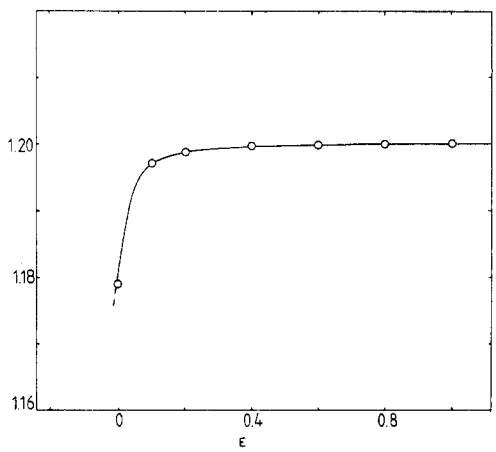

Figure 1. Plot of the last iterate of the sequence $\rho_M(\varepsilon)$ (equation (3.2)) for $1/\nu$ as a function of the shift parameter ε.

This is a considerable improvement on the estimate of $1/\nu \simeq 1.19 \pm 0.03$ obtained by Roomany *et al* (1980).

The same sequence transformations (2.17) can also be applied to the Roomany–Wyld approximants β_M^{RW} defined by (2.15) to obtain an accurate estimate of the β function of the infinite system over the whole of the strong-coupling range $0 \leqslant \lambda \leqslant 1$. This function is shown in figure 2. The slope at the critical point is $-(2\lambda_c \nu)^{-1}$, which yields $1/\nu$ very close to 1.2, in agreement with the more accurate estimate (3.4).

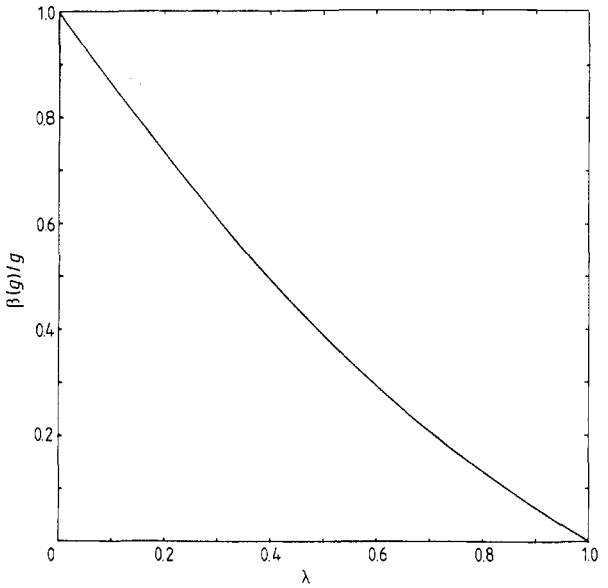

Figure 2. The Callan–Symanzik function $\beta(g)/g$ plotted against λ for the Z_3 model. The curve was obtained by sequence extrapolation from the Roomany–Wyld finite-lattice estimates. Expected errors are less than the width of the line.

3.3. Susceptibility and specific heat

Estimates of the exponent ratio γ/ν follow from the susceptibility. Using the same analysis as described above, we find that the 'best' extrapolation occurs for $\varepsilon \simeq -0.4$, whence we obtain (see table 4)

$$\gamma/\nu = 1.733 \pm 0.001. \tag{3.5}$$

The specific heat presents special problems. While (2.13) remains valid in the limit $M \to \infty$, one also expects a 'regular' background. Thus the asymptotic behaviour

$$C_M(\lambda_c) = AM^{\alpha/\nu} + B + o(1), \qquad M \to \infty, \tag{3.6}$$

is probably a better form to fit finite-lattice data. In view of (3.6), the sequence $(M+\varepsilon)[C_M(\lambda_c) - C_{M-1}(\lambda_c)]/C_M(\lambda_c)$ approaches α/ν as $O(M^{-\alpha/\nu})$. Since we expect $\alpha/\nu \sim 0.4$, the convergence of the table of VBS approximants will be considerably slower (Barber and Hamer 1981) than in the previous cases.

Table 4. VBS approximants for γ/ν for Z_3 model ($\varepsilon = -0.4$).

1.770 40			
1.747 09	1.736 53		
1.739 82	1.734 61	1.733 13	
1.736 79	1.733 89	1.733 32	1.733 01
1.735 30	1.733 60	1.733 85	
1.734 51	1.726 94		
1.733 79			

This is indeed the case, and the best we can do with our previous form of analysis is the estimate

$$\alpha/\nu = 0.40 \pm 0.05. \tag{3.7}$$

The form (3.6) however suggests extrapolating the sequence

$$D_M = C_M(\lambda_c) - C_{M-1}(\lambda_c) \sim AM^{\alpha/\nu - 1}, \qquad M \to \infty, \tag{3.8}$$

for $\alpha/\nu - 1$. The resulting tables of VBS approximants are better behaved than those to $C_M(\lambda)$ (see e.g. table 5). The region of insensitivity to ε is however rather narrow, and thus as our final estimate we take

$$1 - \alpha/\nu = 0.60 \pm 0.01. \tag{3.9}$$

Combining (3.4), (3.5) and (3.9) yields the final estimates for the critical exponents α, ν and γ themselves, which are given in § 5.

Table 5. VBS approximants to $1-\alpha/\nu$ for Z_3 model ($\varepsilon = -0.2$).

0.887 05			
0.677 73	0.616 64		
0.630 44	0.603 87	0.596 58	
0.613 43	0.599 92	0.599 70	0.599 94
0.605 90	0.599 72	0.599 92	0.599 97
0.602 51	0.594 58	0.596 36	
0.600 13	0.598 74		
0.599 25			

3.4. Other extrapolation procedures

Since the use of VBS approximants is new, it seems worthwhile to make some comparison with other extrapolation techniques (see also Barber and Hamer 1981). As a test case, we use the susceptibility data presented above.

The simplest way to estimate the susceptibility index (see e.g. Hamer and Barber 1981a) is to plot $\ln \chi_M$ against $\ln M$, and fit a straight line to the data whose slope should be γ/ν. Applying this method to the Z_3 susceptibility data, we find $\gamma/\nu \simeq 1.78$. This crude technique takes no account of finite-lattice corrections, and the accuracy of the result is correspondingly low.

An alternative method is to regard the finite-lattice data as terms in a power series

$$G(z) = \sum_{M=0}^{\infty} \chi_M z^M \tag{3.10}$$

where we take $\chi_0 = 1$. Equation (2.13) then implies that

$$G(z) \sim (1-z)^{-\gamma/\nu - 1}, \qquad z \to 1. \tag{3.11}$$

Hence one should be able to estimate $(\gamma/\nu + 1)$ from Padé approximants to $(1-z)\,\mathrm{d}[\ln G(z)]/\mathrm{d}z$ evaluated at $z = 1$. These values are listed in table 6; they suggest

$$\gamma/\nu = 1.75 \pm 0.02, \tag{3.12}$$

which is consistent with (3.5).

Table 6. $[L, M]$ Padé approximants to $(1-z)\,\mathrm{d}[\ln G(z)]/\mathrm{d}z$ evaluated at $z=1$.

M \ L	2	3	4
2	2.422	2.789	2.737
3	2.554	2.757	2.731
4	2.329	2.744	

It can be seen that the accuracy of the VBS approximant result compares favourably with alternative methods. This suggests that VBS approximants may provide an important new technique in the extrapolation of sequences and series (see also Barber and Hamer 1981).

4. Results for Z_5 model

There has been some debate about the phase structure of the Z_5 model. In their original paper, EPS showed† that for large enough p values, the Z_p models must have a three-phase structure with a central, massless phase delimited by a dual pair of critical points in λ. From a strong-coupling perturbation expansion, they argued that this was already true for $p=5$, and estimated the strong-coupling critical point to lie at $\lambda_c \simeq 0.92$ for that model. At this point, the mass gap is expected to vanish as

$$F(\lambda) \sim \exp[-b/(\lambda_c - \lambda)^{\sigma}], \tag{4.1}$$

where EPS estimated $\sigma \simeq 0.22$ in contrast to the accepted Kosterlitz (1974) value of $\sigma = \frac{1}{2}$ which applies to the O(2) model and apparently to Z_p models with $p > 5$ (EPS).

More recently, Roomany and Wyld (1981) have performed a finite-lattice analysis of the Z_5 model. They concluded that the critical point lay at $\lambda_c \simeq 0.97$ but that the transition was of the conventional second-order type with the mass gap vanishing algebraically in $\lambda_c - \lambda$ with $\nu \simeq 2.4$.

We have calculated the Z_5 Hamiltonian eigenvalues as functions of λ and h for lattices of up to five sites and as functions of λ alone up to seven sites. Again periodic boundary conditions were applied.

In order to estimate the critical point and to obtain a qualitative picture of the critical behaviour, we first look at the scaled mass gap ratios $R_M(\lambda)$ which are depicted for $M=2$ to 5 in figure 3. It can be seen that these ratios all pass through unity at a steadily increasing sequence of positions λ_M. They do not, however, seem to be converging towards a finite limiting *slope* as they pass through unity, as one would expect for a conventional critical point (Hamer and Barber 1980, 1981a). Rather, the slope decreases as M increases, suggesting that it will go to zero as $M \to \infty$. This behaviour is similar to that found in the O(2) model (Hamer and Barber 1981b) and is suggestive of the expected Kosterlitz–Thouless transition.

Assuming that the critical point estimates λ_M converge logarithmically as usual, and applying the VBS approximants, we obtain a 'best' estimate for λ_c of

$$\lambda_c = 0.990 \pm 0.005 \tag{4.2}$$

† This conclusion has, strictly speaking, only been established for the *Lagrangian* version of the models (see also Wu 1979, Cardy 1980). It is expected to hold also for the Hamiltonian version on universality grounds.

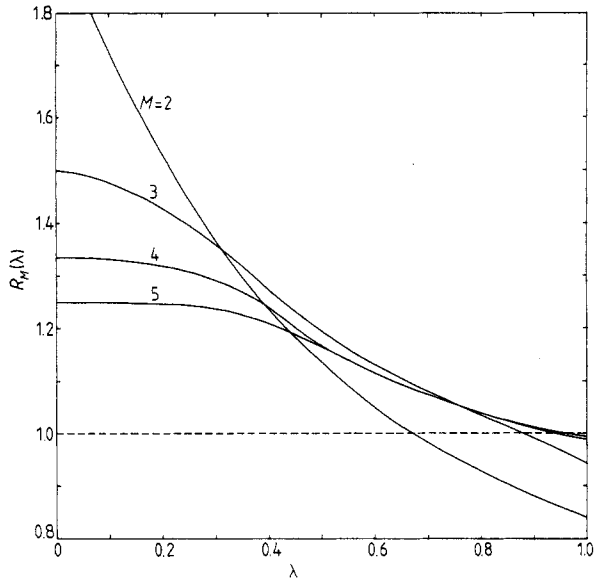

Figure 3. Scaled mass gap ratios $R_M(\lambda)$ for the Z_5 model, plotted against λ for $M = 2, 3, 4$ and 5.

(table 7). Thus the strong-coupling critical point appears to be very close to, but just short of, the self-dual point $\lambda = 1$. This implies a very small region in which the intermediate massless phase exists.

If the mass gap vanishes as in (4.1), then at λ_c the finite-lattice estimates of the β function (2.5) should vary (Hamer and Barber 1981b) as

$$\beta_M(\lambda_c) \sim (\ln M)^{-(1+\sigma)/\sigma}. \tag{4.3}$$

Unfortunately, this result appears to be of little use in exploring the critical behaviour (as was found previously for the O(2) model, Hamer and Barber 1981b).

The Roomany–Wyld approximants β_M^{RW} are however more useful. Extrapolating these via the VBS approximants yields the estimate of the infinite-lattice β function depicted in figure 4. From $\lambda \simeq 0.6$ onwards, this curve is well fitted by a function of the form

$$\beta(g)/g \sim \text{constant}\,(\lambda_c - \lambda)^{1+\sigma}, \tag{4.4}$$

which is implied by (4.1). From the fit (see figure 5) we estimate

$$\sigma = 0.6 \pm 0.1. \tag{4.5}$$

Table 7. VBS approximants to λ_c for Z_5 model ($\varepsilon = 0.0$).

0.669 685		
0.893 611	0.950 904	
0.939 231	0.967 258	0.988 212
0.956 592	0.974 176	0.989 915
0.965 328	0.977 950	
0.970 491		

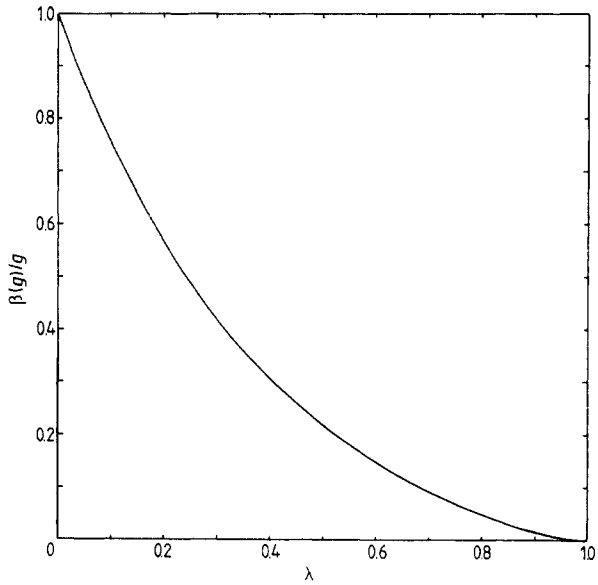

Figure 4. The Callan–Symanzik function $\beta(g)/g$ plotted against λ for the Z_5 model. The curve was obtained by sequence extrapolation from the Roomany–Wyld finite-lattice estimates. Expected errors are of order the width of the line.

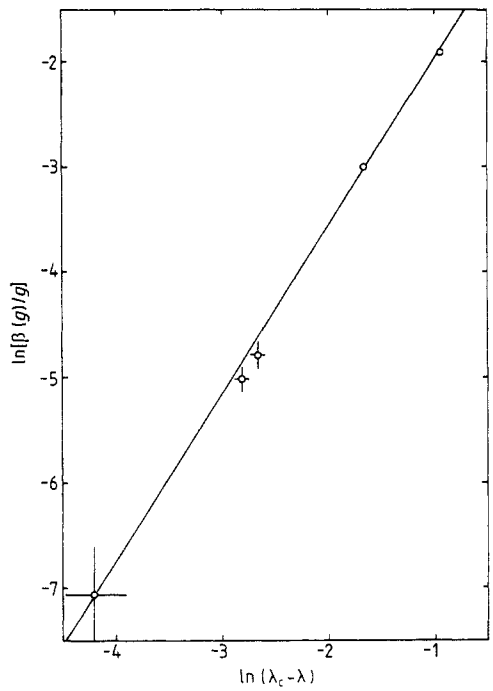

Figure 5. Plot of $\ln[\beta(g)/g]$ against $\ln(\lambda_c - \lambda)$ for the Z_5 model. The data points were obtained by sequence extrapolation from the Roomany–Wyld finite-lattice estimates; and a straight-line fit is shown.

This value is larger than that estimated by EPS and consistent with the 'standard' Kosterlitz–Thouless value of 0.5.

The finite-lattice results for the specific heat are shown in figure 6(a), together with an estimate of their bulk limit obtained again using the VBS approximants. The specific heat shows no sign of a singularity at the critical point. Indeed, there is relatively little size dependence, a good indication of the absence of a critical singularity. Again this behaviour is similar to that observed in the O(2) model.

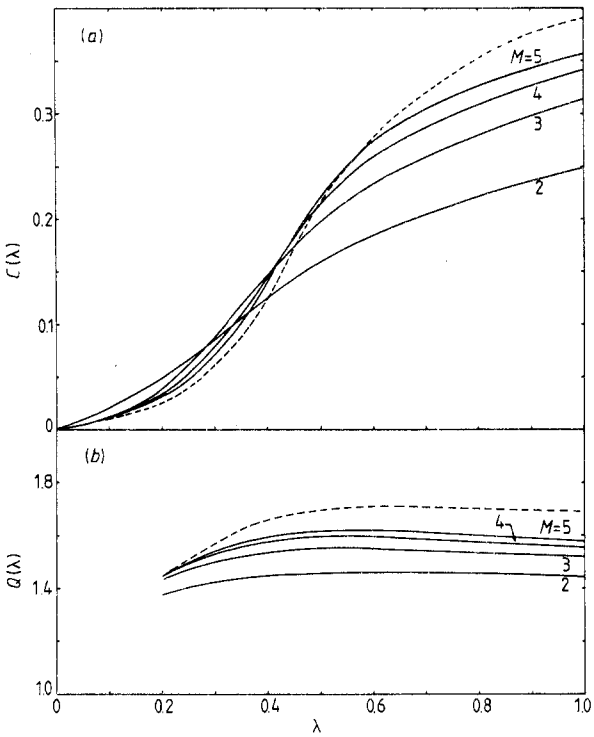

Figure 6. Diagrams of (a) the specific heat $C(\lambda)$, and (b) the quantity $Q(\lambda) \equiv \ln[\chi_M(\lambda)/\lambda^2]/\ln[F_M(\lambda)]$, plotted against λ for the Z_5 model. The full lines are finite-lattice results, labelled by the lattice size M; the broken lines are estimates of the bulk limit, obtained by sequence extrapolation. The errors in these estimates are probably 5–10%.

Finally, in figure 6(b), we plot values of $\ln[\chi_M(\lambda)/\lambda^2]/\ln[F_M(\lambda)]$, where $\chi_M(\lambda)$ is the susceptibility. The curve for the bulk limit was again estimated using VBS approximants. At λ_c, this curve yields an estimate of the exponent η via the result (Hamer and Kogut 1979, 1980)

$$\lim_{\lambda \to \lambda_c} \{\ln[\chi_M(\lambda)/\lambda^2]/\ln F_M(\lambda)\} = 2 - \eta. \tag{4.6}$$

From figure 6(b) we thus obtain the estimate

$$2 - \eta = 1.7 \pm 0.1, \tag{4.7}$$

which is consistent with $\eta = \frac{1}{4}$. However, our sequence is too short for the VBS approximants to provide an accurate quantitative estimate.

5. Summary and conclusions

Our object in this paper was to investigate the use of sequence extrapolation techniques in conjunction with finite-size scaling methods (Fisher and Barber 1972, Hamer and Barber 1980) in order to obtain accurate estimates of the critical parameters of the bulk system from finite-lattice data. The particular sequence transformation we used to accelerate the convergence of the finite-lattice data is due originally to Vanden Broeck and Schwartz (1979), who introduced a general family of such transformations defined by (2.17). This family depends on a set of free parameters (see (2.17)), and we have for the most part specified these by (2.21) (see also Barber and Hamer 1981). Combined with a 'shifting' procedure (see § 3.2), we have found these techniques, overall, to work remarkably well.

The results obtained for the two particular models investigated were as follows.

(a) *Z_3 model*

The EPS conclusion (Elitzur *et al* 1979) was confirmed with high accuracy: the Z_3 or three-state Potts model has a two-phase structure, with a conventional critical point at the self-dual coupling of $\lambda = 1$. The critical exponents α, γ and ν were estimated to be

$$\nu = 0.8333 \pm 0.0003, \qquad \gamma = 1.444 \pm 0.002, \qquad \alpha = 0.33 \pm 0.01.$$

These figures agree with those of previous estimates of these exponents by alternative methods (see Hamer and Kogut (1980) for a summary and comparison of previous calculations), but are at least an order of magnitude more accurate. They are in excellent agreement with the hypothesis (Alexander 1975) that the Z_3 (or three-state Potts) model lies in the same universality class as the 'hard hexagon' model solved recently by Baxter (1980). This means that the critical exponents should be the same for both models, namely $\nu = \frac{5}{6}$, $\gamma = \frac{13}{9}$ and $\alpha = \frac{1}{3}$. Our results leave little room for doubt that this hypothesis is correct (see also Nienhuis *et al* 1980, Hamer and Kogut 1980, Kogut *et al* 1980).

(b) *Z_5 model*

Here we agree with Elitzur *et al* (1979) and disagree with Roomany and Wyld (1981), in concluding that the model has a three-phase structure with an exponential, Kosterlitz–Thouless type phase transition at the two dual critical points. We find the critical point in the strong-coupling region to be $\lambda_c = 0.990 \pm 0.005$, just short of the self-dual point $\lambda = 1$. The central massless phase is thus very small, if indeed it exists at all. We find a value for the exponential critical index σ (recall (4.1)) of $\sigma = 0.6 \pm 0.1$, consistent with the standard Kosterlitz value of $\frac{1}{2}$. Thus our quantitative results differ quite substantially from the EPS results of $\lambda_c \simeq 0.92$ and $\sigma \simeq 0.22$, obtained via a strong-coupling series analysis.

These results for the Z_3 and Z_5 models suggest that the combination of convergence acceleration methods with finite-size scaling yields a powerful tool for the investigation of critical behaviour. By forming a sequence of finite-lattice estimates for some quantity at the expected critical point, one is able to 'sit on top of' the singularity of interest and eliminate all unphysical singularities which tend to bedevil the conventional series techniques. The finite-lattice sequences display smooth and regular convergence, and we have found that no particular difficulties arise even when confluent singularities are expected as in the Z_3 model. (In contrast, see Kogut *et al* (1980) who analyse in detail the perturbation series for Z_3.) These methods should be very useful for all sorts of two-dimensional lattice models, both in statistical mechanics and field theory.

In higher dimensions the utility of the methods is less clear. Because of simple counting problems caused by the rapid increase of sites with the linear dimension of the lattice, it becomes much more difficult actually to compute the Hamiltonian eigenvalues on a sequence of lattices of reasonable size. If the finite-lattice sequences are too short, the sequence extrapolation procedures will be of limited use. Nevertheless, preliminary investigations (Roomany and Wyld (1980), who studied Z_2 in $(2+1)$ dimensions) suggest that one may still be able at least to obtain reliable qualitative pictures of a model's behaviour from finite lattices of extremely small size.

Appendix. Comparison of numerical methods

Methods for the numerical computation of Hamiltonian eigenvalues on a finite lattice have been discussed in previous works (Hamer and Barber 1981b, Roomany *et al* 1980). We refer to these for background material.

There are two main stages to the calculation.

Stage 1. Construction of a set of orthonormal basis states on the finite lattice, and calculation of the matrix elements H_{ij} connecting them. Here

$$H = H_0 + \lambda V. \tag{A1}$$

One starts from an eigenstate of H_0, and constructs further basis states by successive applications of the operator V (see references above).

Stage 2. Calculation of the eigenvalues of the matrix $[H_{ij}]$. Standard library subroutines are available for this part of the calculation.

We have used two different methods for our calculations.

(A) One of us (CJH) catalogued each individual spin configuration as a separate basis state, held in a single, address-sorted, master file at stage 1. Successive applications of V rapidly build up a *complete* set of basis states for Z_3 and Z_5 models on a finite lattice. Stage 2 was then performed by an iterative method, for each desired parameter value, and to any desired level of accuracy.

Advantages of the method are the saving of storage space, since each configuration is only stored once, and no coefficients are needed; and efficient generation of basis states, since each spin configuration need only be processed (by application of V) once. The disadvantage is that the calculation of eigenvalues (stage 2) is slow because of the large number of basis states.

(B) The other author (MNB) used the Lanczos technique (Paige 1972, Hamer and Barber 1981b, Roomany *et al* 1980). Details of this method may be found in the references above. The great advantage of this method is that the Hamiltonian is brought to a tridiagonal form, on relatively few basis states, so that stage 2 is very quick. Disadvantages are that the basis states contain large numbers of spin configurations, each with different coefficients, so that large amounts of storage space are required. Numerical accuracy has to be carefully watched; and stage 1 of the calculation has to be repeated, at least in part, for each different set of parameter values (because the coefficients of the spin configurations depend on the parameters).

Thus method (B) is more laborious at stage 1, but much quicker at stage 2. We tend to favour method (A) because it is easier to obtain high accuracy, and because as one goes to higher dimensions stage 1 of the calculations becomes very much more difficult.

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