Magnetisations from finite-size scaling

1982 J. Phys. A: Math. Gen. 15 L675

(http://iopscience.iop.org/0305-4470/15/12/005)

J. Phys. A: Math. Gen. **15** (1982) L675–L683. Printed in Great Britain

LETTER TO THE EDITOR

Magnetisations from finite-size scaling

C J Hamer

Department of Theoretical Physics, Research School of Physical Sciences, The Australian National University, PO Box 4, Canberra ACT 2600, Australia

Received 14 September 1982

Abstract. A method of obtaining the spontaneous magnetisation from finite-lattice matrix elements of the magnetic field operator, due to Yang and Uzelac, is discussed. The method is demonstrated for the case of the Ising model in $(1+1)$ dimensions, and is shown to provide smooth and rapidly convergent finite-lattice sequences. Applied to the case of the three-state Potts (Z_3) model in $(1+1)$ dimensions, the method yields an estimate $\beta = 0.111\,09 \pm 0.000\,05$ for the critical exponent. This confirms Alexander's conjecture of universality with the hard hexagon model.

The spontaneous magnetisation of a spin model in zero magnetic field is difficult to calculate by finite-size scaling methods (Fisher 1971, Fisher and Barber 1972, Barber 1982). The problem is that on a finite lattice the spontaneous magnetisation always vanishes: the ground state is rotationally symmetric in zero magnetic field. It is only in the bulk limit that spontaneous symmetry breaking occurs.

One may try to proceed by a double limiting process: that is, by calculating the magnetisation in non-zero field h, then taking the lattice size to infinity (bulk limit), and then taking the limit $h \to 0$. This process will, in principle, yield the correct spontaneous magnetisation. But the double limit is a delicate one, since the convergence is non-uniform, and one must be careful to take the bulk limit and the zero-field limit in the order specified. In practice, one cannot expect to achieve very good accuracy by such a procedure (Hamer 1981).

The solution to this problem was pointed out long ago by Yang (1952), and has been rediscovered recently by Uzelac (1980) in the context of finite-size scaling theory (or the 'phenomenological renormalisation group', cf Nightingale (1977)). Consider, for example, the quantum field theory version of the 2D Ising model.† The quantum Hamiltonian for this model, in a low-temperature representation, is (Fradkin and Susskind 1978)

$$H = \sum_{m=1}^{M} \{[1 - \sigma_3(m)\sigma_3(m+1)] - \lambda' \sigma_1(m) + h\sigma_3(m)\} \tag{1}$$

where the index m labels sites on a one-dimensional spatial lattice, and the $\sigma_i(m)$ are Pauli matrices acting on a two-state spin variable at each site. The coupling λ' acts as a temperature variable, and h is the magnetic field. The two leading (lowest-energy) eigenvectors of this Hamiltonian may be denoted $|1+\rangle$ and $|2-\rangle$, respectively, where

† The following argument extends immediately to the ordinary Euclidean framework of statistical mechanics if one everywhere replaces 'quantum Hamiltonian' by (minus the) 'logarithm of the transfer matrix' (Fradkin and Susskind 1978, Kogut 1979).

the signs refer to the symmetry of each state under a reversal of all spins. For λ' less than the critical temperature $\lambda_c' = 1$, and for $h = 0$, these two states become degenerate in the bulk limit.

Now consider the effect of a very small magnetic field h on these two states. Let the matrix element of the magnetic field term between them be

$$\alpha = \left\langle 2- \left| \sum_{m=1}^{M} \sigma_3(m) \right| 1+ \right\rangle. \tag{2}$$

Then the effect of this small perturbation is to *mix* the two degenerate states, and thus to produce a spontaneous breakdown of the spin reversal symmetry. The new ground-state energy, to leading order in h, is the minimum eigenvalue of the 2×2 matrix

$$\begin{pmatrix} E_0 & h\alpha \\ h\alpha & E_0 \end{pmatrix} \tag{3}$$

where E_0 is the unperturbed eigenvalue; hence the spontaneous magnetisation (Hamer and Kogut 1980) is

$$\mathcal{M}(h=0) \equiv \lim_{\substack{M\to\infty \\ h\to 0}} \left(\frac{1}{M} \frac{\mathrm{d}E_0(h)}{\mathrm{d}h} \right) = \frac{\alpha}{M} = \langle 2- |\sigma_3(1)| 1+ \rangle. \tag{4}$$

The last equality follows from translational invariance of the ground state. A more rigorous demonstration of this result may be found in Schultz *et al* (1964).

Now the relation (4) depends on the exact degeneracy of the states $|1+\rangle$ and $|2-\rangle$, and is therefore only true in the bulk limit $M \to \infty$. On a finite lattice, the quantity $\mathrm{d}E_0/\mathrm{d}h$ is zero at $h = 0$, as we have seen, and is consequently useless for estimating the spontaneous magnetisation. But the matrix element α/M is *not* zero at $h = 0$, and in fact provides a smooth sequence converging to the bulk spontaneous magnetisation as the lattice size $M \to \infty$. Our problem is therefore solved.

To demonstrate this, we apply the idea to the Z_2 (Ising) and Z_3 (three-state Potts) models in $(1+1)$ dimensions. The quantum Hamiltonian for the Z_p model is (Elitzur *et al* 1979)

$$H(\lambda, h) = -\sum_{i=1}^{M} [\cos(2\pi L_i/p) + \tfrac{1}{2}\lambda (R_i^+ R_{i-1}^- + R_i^- R_{i-1}^+) - \tfrac{1}{2}h(R_i^+ + R_i^-)], \tag{5}$$

where we apply periodic conditions so that $R_{M+i}^{\pm} = R_i^{\pm}$. In the high-temperature representation, which we shall employ here, 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 at site i. The parameter λ is an inverse temperature, and h is the magnetic field. For the case $p = 2$, the Hamiltonian (5) is equivalent to (1).

The Z_p models are self-dual: the Hamiltonian (5) satisfies the relation (Elitzur *et al* 1979)

$$H(\lambda) = \lambda H(1/\lambda). \tag{6}$$

Hence in the cases where there is a single second-order phase transition (i.e. cases $p = 2, 3, 4$), the critical point must lie at $\lambda_c = 1$.

The generalisation of the argument given above for the special case of the Ising model is immediate. For temperatures below the critical point, the Z_p model has p degenerate ground states at $h = 0$; and the 2×2 matrix (3) is replaced by a cyclic,

tridiagonal, $p \times p$ matrix. It is easily shown that the finite-lattice 'magnetisation' is equal to the largest eigenvalue of the matrix $\{\langle i|R_1^+ + R_1^-|j\rangle\}$, where the states $\{|i\rangle\}$ are the p ground states.

In the high-temperature representation (5), the spectrum at $h = 0$ breaks up into p disjoint sectors, each characterised by an eigenvalue of $(\Sigma_{i=1}^{M} L_i) \bmod p$. The ground state in each of these sectors becomes one of the p degenerate ground states in the bulk limit, at low temperatures.

The computation then proceeds via standard methods (Hamer and Barber 1980, 1981a, b). For each lattice size M, a matrix Hamiltonian is generated using the high-temperature spin eigenstates as a basis. At each coupling value λ, the ground state of this Hamiltonian in each of the p sectors can then be calculated using an iterative method. We used a conjugate gradient method for this purpose, rather than the Lanczos method, in the belief that the former gives the more reliable estimates of the eigenvectors. Having found the p ground-state eigenvectors, it is easy to compute the matrix elements of the magnetic field operator between them, and hence the finite-lattice 'magnetisation', as defined above. We have computed these matrix elements to an accuracy of order 1 part in 10^9.

The first case to consider is $p = 2$, the Ising model, where one may compare our numerical answers with known exact results. We have computed the finite-lattice 'magnetisations' for a sequence of lattice sizes $M = 1, 2, \ldots, 13$. Below the critical point, it is found that the finite-lattice estimates form a smooth and rapidly convergent sequence. An example is shown in table 1, for the coupling $\lambda^{-1} = 0.8$. The convergence of the sequence has been accelerated using a Padé table†, appropriate to the expected 'linear' convergence (Hamer and Barber 1981b). The rightmost entry in the table should be compared with the exact result (Pfeuty 1970)

$$\mathcal{M}(\lambda) = (1 - \lambda^{-2})^{1/8} = 0.880\,111\,737 \qquad \text{at } \lambda^{-1} = 0.8. \tag{7}$$

It can be seen that the two figures agree within 1 part in 10^8, and that the use of the sequence transformation table has improved the accuracy of the result by five significant figures.

One may now apply finite-size scaling techniques to estimate the critical index β. The standard scaling assumption (Uzelac and Jullien 1981, Hamer and Barber 1981a) for the finite-lattice 'magnetisation' at the critical point $\lambda_c = 1$ will be

$$\mathcal{M}_M(\lambda_c) \underset{M\to\infty}{\sim} \text{constant}\, M^{-\beta/\nu}. \tag{8}$$

Hence the exponent ratio β/ν can be estimated as the limit of the sequence

$$\rho_M(\varepsilon) = (M + \varepsilon)[\mathcal{M}_M(\lambda_c)/\mathcal{M}_{M-1}(\lambda_c) - 1], \tag{9}$$

since the scaling relation (8) implies

$$\lim_{M\to\infty} \rho_M(\varepsilon) = -\beta/\nu \qquad \text{for all } \varepsilon. \tag{10}$$

The 'end-shift' ε is a free parameter, introduced to check the stability and accuracy of the result (Hamer and Barber 1981b). The finite-lattice values $\mathcal{M}_M(\lambda_c)$ are listed for the Ising (Z_2) model in the first column of table 2; and from these the sequence $\{\rho_M(\varepsilon)\}$ was computed. The convergence of this sequence was accelerated using an

† Generated using the Vanden Broeck and Schwartz (1979) algorithm, with parameter $\alpha = 1$.

Table 1. Table of VBS approximants ($\alpha = 1$) to the Ising model 'magnetisation' for $\lambda^{-1} = 0.8$. The left-hand column consists of successive finite-lattice results, for $M = 1$ to 13.

M							
1	1.000 000 000						
2	0.943 628 319	0.893 935 608					
3	0.917 217 366	0.885 286 366	0.880 913 349				
4	0.902 762 448	0.882 091 218	0.880 295 723	0.880 122 242			
5	0.894 255 938	0.880 874 003	0.880 149 234	0.880 109 807	0.880 109 480		
6	0.889 055 315	0.880 403 762	0.880 116 777	0.880 109 486	0.880 109 711	0.880 111 972	
7	0.885 807 199	0.880 221 795	0.880 110 697	0.880 110 171	0.880 112 729	0.880 111 750	0.880 111 733
8	0.883 753 427	0.880 151 950	0.880 110 211	0.880 110 438	0.880 111 804	0.880 111 734	
9	0.882 445 507	0.880 125 633	0.880 110 632	0.880 123 811	0.880 111 742		
10	0.881 609 128	0.880 116 039	0.880 111 029	0.880 111 900			
11	0.881 073 045	0.880 112 740	0.880 111 288				
12	0.880 729 015	0.880 111 731					
13	0.880 508 104						

Table 2. Finite-lattice results for the 'magnetisations' $\mathcal{M}_M$ at $\lambda = \lambda_c = 1$ for the Z_2 and Z_3 models, as a function of lattice size M.

M	$\mathcal{M}_M$ (Z_2 model)	$\mathcal{M}_M$ (Z_3 model)
1	1.000 000 000	1.000 000 000
2	0.923 879 533	0.925 572 723
3	0.879 652 811	0.881 242 391
4	0.849 088 295	0.850 237 673
5	0.825 964 093	0.826 608 472
6	0.807 477 524	0.807 624 549
7	0.792 141 322	0.791 819 587
8	0.779 076 491	0.778 319 387
9	0.767 722 363	0.766 562 595
10	0.757 700 394	0.756 168 177
11	0.748 743 497	
12	0.740 656 483	
13	0.733 292 558	

'alternating VBS transformation' (Vanden Broeck and Schwartz 1979, Hamer and Barber 1981b), appropriate to the expected 'logarithmic' convergence at the critical point.

The resulting estimates of β/ν are plotted against ε in figure 1(a). The results become unstable around $\varepsilon \simeq -0.3$, as the sequence switches between convergence from above and convergence from below. Choosing a value $\varepsilon = -1.0$, well away from this instability, we obtain the VBS table given in table 3. From this table, and figure 1(a), we may conclude

$$\beta/\nu = 0.125\,00 \pm 0.000\,01, \tag{11}$$

which is in excellent agreement with the exact result (Yang 1952), $\beta/\nu = \frac{1}{8}$. The accuracy of our result appears to be limited by round-off error, in fact, rather than the finite length of the sequence $\{\rho_M(\varepsilon)\}$.

Next, the same techniques were applied to the Z_3 or three-state Potts model. The 'magnetisations' were computed for a sequence of lattice sizes $M = 1, 2, \ldots, 10$, the latter case involving a total of 3210 high-temperature basis states. The qualitative behaviour of the magnetisation estimates was very similar to the Ising model case. Table 2, column 2, lists the finite-lattice values of $\mathcal{M}(\lambda_c)$. Figure 1(b) graphs the variation of the β/ν estimate against ε; and table 4 contains the VBS table for the case $\varepsilon = -1.0$. We conclude

$$\beta/\nu = 0.133\,31 \pm 0.000\,03; \tag{12}$$

and hence, using our previous estimate (Hamer and Barber 1981b) $\nu^{-1} = 1.2000 \pm 0.0005$, one finds

$$\beta = 0.111\,09 \pm 0.000\,05. \tag{13}$$

These results should be compared with the universality hypothesis (Alexander 1975) that the three-state Potts model should have the same exponent as the 'hard hexagon' model solved by Baxter (1980), namely $\beta = \frac{1}{9} = 0.1111\ldots$. There seems little room for doubt that this hypothesis is correct. Conventional series analyses have not been accurate enough to check this conclusion: results in the ordinary Euclidean

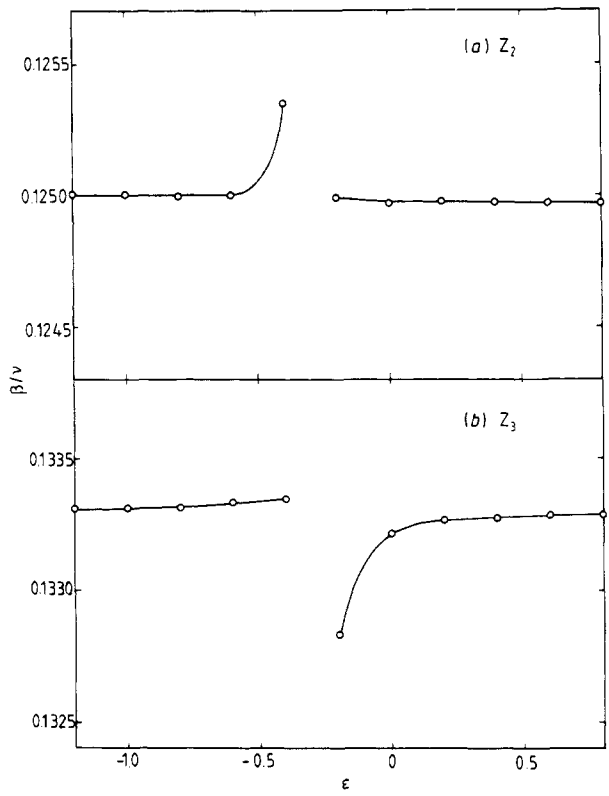

Figure 1. Plot of the last VBS approximant to β/ν (obtained from the sequence $\rho_M(\varepsilon)$), as a function of the end-shift parameter ε. (*a*) shows results for the Z_2 model; (*b*) is for the Z_3 model.

framework, reviewed by Wu (1982), have ranged between 0.106 and 0.109 for β, while in the Hamiltonian field theory version, a result $\beta = 0.108 \pm 0.002$ was obtained (Hamer and Kogut 1980). But recently these magnetisation series have been re-analysed by Adler and Privman (1982) using a method that explicitly accounts for the effect of confluent corrections to scaling. They obtain greatly improved estimates, namely

$$\begin{aligned} &\beta = 0.1110 \pm 0.0007 \qquad \text{(Euclidean statistical mechanics)} \\ &\beta = 0.1111 \pm 0.0006 \qquad \text{(Hamiltonian field theory).} \end{aligned} \tag{14}$$

These results are in excellent agreement with ours.

In summary, then, we have studied a method due to Yang (1952) and Uzelac (1980) of estimating spontaneous magnetisations from matrix elements of the magnetic field operator on a finite lattice. The method has been demonstrated for the case of the Ising (Z_2) model in $(1+1)$ dimensions, and has been found to provide a smooth and rapidly convergent finite-lattice sequence. This allows estimates of the magnetisation and its critical index of excellent accuracy. Applied to the three-state Potts (Z_3) model, the method yields critical exponent estimates $\beta/\nu = 0.133\,31 \pm 0.000\,03$, $\beta = 0.111\,09 \pm 0.000\,05$. These are in excellent agreement with the series results of Adler

Table 3. Alternating VBS approximants to β/ν for the Z_2 model. The left-hand column lists successive values of the sequence $-\rho_M(\varepsilon)$, at $\varepsilon = -1.0$, for lattice sizes $M = 2, 3, \ldots, 13$.

M						
2	0.076 120 468					
3	0.095 741 316	0.110 728 864				
4	0.104 238 341	0.114 747 424	0.125 339 886			
5	0.108 936 617	0.117 028 404	0.125 131 401	0.125 037 810		
6	0.111 909 038	0.118 487 404	0.125 066 807	0.125 017 668	0.125 010 329	
7	0.113 956 374	0.119 498 113	0.125 038 899	0.125 012 820	0.125 019 345	0.125 013 447
8	0.115 451 392	0.120 238 671	0.125 025 417	0.125 001 875	0.125 002 291	0.125 001 823
9	0.116 590 636	0.120 804 241	0.125 016 845	0.125 002 316	0.125 001 835	
10	0.117 487 415	0.121 250 104	0.125 011 454	0.125 010 759		
11	0.118 211 596	0.121 610 534	0.125 010 839			
12	0.118 808 583	0.121 907 907				
13	0.119 309 152					

Table 4. Alternating VBS approximants to β/ν for the Z_3 model. The left-hand column lists successive values of the sequence $-\rho_M(\varepsilon)$, at $\varepsilon = -1.0$, for lattice sizes $M = 2, 3, \ldots, 10$.

M					
2	0.074 427 277				
3	0.095 790 057	0.113 755 978			
4	0.105 548 885	0.118 779 418	0.133 914 174		
5	0.111 165 157	0.121 714 356	0.133 502 485	0.133 349 032	
6	0.114 830 201	0.123 636 148	0.133 390 699	0.133 323 529	0.133 310 712
7	0.117 418 142	0.124 994 063	0.133 348 741	0.133 315 960	
8	0.119 347 136	0.126 006 092	0.133 330 338		
9	0.120 842 847	0.126 790 516			
10	0.122 038 002				

and Privman (1982), and provide confirmation for Alexander's hypothesis of universality with the hard hexagon model; they also confirm the universality between the ordinary statistical mechanics version and the Hamiltonian field theory version of the model. We may note that no special allowance was necessary for confluent corrections to scaling in the finite-lattice method: such corrections will merely alter the rate of 'logarithmic' convergence at the critical point (Hamer and Barber 1981b).

It should be possible to generalise this method in order to obtain the order parameter or latent heat at any first-order transition point. This will depend, however, on a correct identification of the finite-lattice eigenstates which become degenerate in the bulk limit, which is not always an entirely trivial problem.

I would like to thank Dr Alan Irving for some illuminating discussions of the correspondence between the high-temperature and low-temperature representations on a finite lattice.

References

Adler J and Privman V 1982 *J. Phys. A: Math. Gen.* **15** L417
Alexander S 1975 *Phys. Lett.* **54A** 353
Barber M N 1982 *University of New South Wales preprint*
Baxter R J 1980 *J. Phys. A: Math. Gen.* **13** L61
Elitzur S, Pearson R B and Shigemitsu J 1979 *Phys. Rev.* D **19** 3698
Fisher M E 1971 in '*Critical Phenomena*', *Proc. Int. School of Physics 'Enrico Fermi', Varenna 1970, Course No 51* ed M S Green (New York: Academic)
Fisher M E and Barber M N 1972 *Phys. Rev. Lett.* **28** 1516
Fradkin E and Susskind L 1978 *Phys. Rev.* D **17** 2637
Hamer C J 1981 *J. Phys. A: Math. Gen.* **14** 2981
Hamer C J and Barber M N 1980 *J. Phys. A: Math. Gen.* **13** L169
—— 1981a *J. Phys. A: Math. Gen.* **13** 241, 259
—— 1981b *J. Phys. A: Math. Gen.* **14** 2009
Hamer C J and Kogut J 1980 *Phys. Rev.* B **22** 3378
Kogut J 1979 *Rev. Mod. Phys.* **51** 659
Nightingale M P 1977 *Phys. Lett.* **59A** 486
Pfeuty P 1970 *Ann. Phys.* **57** 79
Schultz T D, Mattis D C and Lieb E H 1964 *Rev. Mod. Phys.* **36** 856

Uzelac K 1980 *Thesis, Orsay*
Uzelac K and Jullien R 1981 *J. Phys. A: Math. Gen.* **14** L151
Vanden Broeck J-M and Schwartz L W 1979 *SIAM J. Math. Anal.* **10** 658
Wu F Y 1982 *Rev. Mod. Phys.* **54** 235
Yang C N 1952 *Phys. Rev.* **85** 808