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Cluster expansions for the Ising and Heisenberg spin models in Hamiltonian lattice field theory

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Abstract. Cluster expansion methods are applied to calculate 'high-temperature' series for the vacuum energy, the susceptibility and the mass gap for the Ising model and the O(2) and O(3) Heisenberg models in $(1+1)$ dimensions and $(2+1)$ dimensions. Critical points and critical indices are estimated for the line, the square and the triangular lattices. The results demonstrate universality with the normal Euclidean versions of these models, within errors.

1. Introduction

Analysis of high-temperature series is one of the most accurate ways to estimate critical parameters for a lattice spin model (see, e.g., Gaunt and Guttmann 1974, Guttmann 1989). In this paper, we use the cluster expansion methods of Nickel (1980) to calculate high-temperature series for the Ising and Heisenberg spin systems in their Hamiltonian lattice field theory versions.

The linked cluster expansion method suggested by Nickel (1980) is the most efficient technique known for generating perturbation series in lattice Hamiltonian field theory. The idea is perhaps most easily understood in diagrammatic terms. Each term in the perturbation series for the ground-state energy, for instance, can always be associated with a diagram of an appropriate type; and because the ground-state energy is an extensive quantity, it can be expressed in terms of connected diagrams alone. Each diagram spans a connected set of sites on the underlying spatial lattice, called a 'linked cluster'. The algorithm then runs as follows. A list is generated of the possible linked clusters up to some maximum size, together with their lattice constants. The ground-state energy is calculated for each cluster, and the contributions from all the smaller embedded sub-clusters are subtracted out, leaving only the 'intrinsic' terms corresponding to diagrams which completely span the original cluster. Multiplying by the lattice constant, one obtains the contribution of this set of diagrams to the bulk ground-state energy per site. More detailed descriptions of these methods have been given in earlier papers (Marland 1981, Irving and Hamer 1984, Hamer and Irving 1984), and will not be repeated here.

The resulting series extend those previously available for these models. We analyse them using eight different methods of series analysis, as discussed in § 3. The results of this analysis appear to give the best series estimates to date of the susceptibility exponent γ and the critical point x_c, though for the correlation-function exponent η earlier results based on finite-size scaling appear to offer greater accuracy. In each

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case however, a satisfying consistency with the Euclidean lattice model results is obtained.

In § 2 of the paper the quantum Hamiltonians for these models are set down, and the series coefficients are presented. In § 3 we describe the analysis of these series, and our conclusions are summarised in § 4.

2. Series generation

The quantum Hamiltonian of the lattice field theory version of the Ising model is (Fradkin and Susskind 1978)

$$H = \sum_i (1 - \sigma_3(i)) - x \sum_{\langle ij \rangle} \sigma_1(i)\sigma_1(j) - h \sum_i \sigma_1(i) \tag{2.1}$$

where the index i labels sites on a spatial lattice and $\langle ij \rangle$ are nearest-neighbour pairs of sites, while the time variable is continuous. The σ_k are Pauli matrices acting on a two-state spin variable at each site, x is the coupling (corresponding to the inverse temperature β in the Euclidean formulation), and h is a magnetic field variable. The second and third terms in equation (2.1) are exactly the same spatial interaction terms which appear in the ordinary Euclidean Hamiltonian; while the first term is the remnant of the pairwise interaction in the 'time' direction which survives after taking the 'τ-continuum' limit (Fradkin and Susskind 1978).

We have calculated perturbation series for the lowest two eigenvalues ω_0 and ω_1 of the Hamiltonian (2.1). Quantities derived therefrom are: the ground-state energy per site ω_0/N, where N is the number of sites of the lattice; the mass gap

$$F(x) = \omega_1(x) - \omega_0(x) \tag{2.2}$$

and the magnetic susceptibility

$$\chi(x) = -\frac{1}{N} \frac{\partial^2 \omega_0}{\partial h^2}\bigg|_{h=0}. \tag{2.3}$$

Table 1 lists coefficients of the perturbation series in x for each quantity, for the square and triangular lattices. The coefficients were previously calculated to seventh order on the square lattice and to sixth order on the triangular lattice by Hamer and Irving (1984).

The quantum Hamiltonian for the O(2) Heisenberg model is (Hamer *et al* 1979)

$$H = \sum_i J^2(i) - x \sum_{\langle ij \rangle} \boldsymbol{n}(i) \cdot \boldsymbol{n}(j) - h \sum_i n_1(i) \tag{2.4}$$

where $\boldsymbol{n}(i)$ is a two-component spin vector at site i, normalised to unity, so that

$$\begin{aligned} \boldsymbol{n}(i) &\equiv (n_1(i), n_2(i)) \\ &= (\cos\theta(i), \sin\theta(i)) \end{aligned} \tag{2.5}$$

and $J(i)$ is the angular momentum operator conjugate to $\theta(i)$, which can take any integer eigenvalue. If we define

$$\varphi(i) = \exp[\mathrm{i}\theta(i)] = n_1(i) + in_2(i)$$

then $\varphi(i)$, $\varphi^\dagger(i)$ are raising and lowering operators for $J(i)$, obeying commutation relations

$$[J(i), \varphi(j)] = \varphi(i)\delta_{ij} \qquad [J(i), \varphi^\dagger(j)] = -\varphi^\dagger(i)\delta_{ij}. \tag{2.6}$$

Table 1. High temperature series in x for the vacuum energy per site ω_0/N, the susceptibility χ and the mass gap F for the Ising model. Coefficients of x^n are listed for the square and triangular lattices.

n	ω_0/N	χ	F
		Square lattice	
0	0.0	1.0	2.0
1	0.0	4.0	−4.0
2	−0.5	13.5	−2.0
3	0.0	45.0	−3.0
4	−0.468 75	144.843 75	−4.5
5	0.0	464.444 444 44	−11.0
6	−1.148 437 5	1 469.358 506 94	−20.507 812 5
7	0.0	4 639.482 349 54	−57.699 218 7499
8	−4.395 263 671 88	14 544.119 239 7	−114.836 303 711
9	0.0	45 537.479 663 3	−350.106 720 13
		Triangular lattice	
0	0.0	1.0	2.0
1	0.0	6.0	−6.0
2	−0.75	32.25	−6.0
3	−0.75	166.5	−10.5
4	−1.359 375	843.046 875	−31.5
5	−3.093 75	4 218.416 666 67	−98.531 25
6	−8.355 468 75	20 941.023 003 5	−346.710 937 5
7	−24.667 968 75	103 361.512 587	−1255.205 566 41
8	−78.127 358 3008	507 986.371 687	−4795.437 012 0

Table 2 lists the perturbation series coefficients for this model. The susceptibility series for the line lattice was previously calculated to sixth order by Hamer and Kogut (1979), and the mass gap series was obtained to tenth order by Hornby and Barber (1985). Sobelman (1981) has calculated the mass gap to fourth order for a hypercubic lattice in any number of dimensions.

For the O(3) Heisenberg model, the quantum Hamiltonian is

$$H=\sum_i \boldsymbol{J}^2(i)-x\sum_{\langle ij\rangle}\boldsymbol{n}(i)\cdot\boldsymbol{n}(j)-h\sum_i n_1(i) \tag{2.7}$$

where now $\boldsymbol{n}(i)$ is a three-component spin vector at site i (normalised to unity), and $\boldsymbol{J}(i)$ is a vector angular momentum operator. For further detials, we refer to Hamer *et al* (1979). Table 3 lists the perturbation series for this model. For the line lattice, the mass gap series has previously been calculated to sixth order by Hamer *et al* (1979), and the susceptibility series to sixth order by Hamer and Kogut (1979). The (2+1)-dimensional model has not been studied before, to our knowledge.

3. Series analysis

The 24 series listed in tables 1, 2 and 3 have all been analysed by eight distinct methods. Seven of the methods extrapolate the ratios of coefficients, while the eighth method is the method of differential approximants (Guttmann and Joyce 1972, Rehr *et al* 1980). Attempting to extrapolate the ratios of coefficients it is clear that, in most cases,

Table 2. High-temperature series in x for the vacuum energy per site ω_0/N, the susceptibility χ and the mass gap F for the O(2) Heisenberg model. Coefficients of x^n are listed for the line, square and triangular lattices.

n	ω_0/N	χ	F
		Line lattice	
0	0.0	1.0	1.0
1	0.0	2.0	−1.0
2	−0.25	2.6	0.125
3	0.0	2.887 5	0.031 25
4	0.006 510 416 667	2.895 434 138 39	0.014 388 020 833 3
5	0.0	2.696 261 969 00	0.006 002 061 631 94
6	0.001 220 444 775 13	2.394 661 629 47	0.000 226 149 678 417
7	0.0	2.042 744 227 03	0.000 695 799 136 309
8	0.000 018 130 926 5634	1.686 753 325 07	−0.000 175 027 796 25
		Square lattice	
0	0.0	1.0	1.0
1	0.0	4.0	2.0
2	−0.5	13.2	−0.75
3	0.0	42.575	−1.375
4	−0.382 812 5	131.887 566 369	−1.379 817 708 33
5	0.0	404.761 871 477	−4.087 947 048 63
6	−0.718 256 035 053	1 223.918 123 46	−5.678 693 667 86
7	0.0	3 682.463 983 34	−18.405 049 435 9
8	−0.231 359 616 070	10 992.868 315 5	
		Triangular lattice	
0	0.0	1.0	1.0
1	0.0	6.0	−3.0
2	−0.75	31.8	−2.625
3	−0.75	160.222 5	−4.312 5
4	−1.167 968 75	786.990 563 358	−12.065 429 687 5
5	−2.356 770 833 33	3 806.089 606 55	−35.091 933 593 8
6	−5.784 368 024 56	18 214.774 502 4	−116.279 209 828
7	−15.736 769 379	86 508.909 227	−393.768 284
8	−46.094 316 275 8	408 510.254 601	−1421.975 816 67

the ratios are affected by one or more singularities other than the physical singularity—usually an 'antiferromagnetic' singularity on the negative real axis. To diminish the effect of this singularity, we have first transformed the series by an Euler transformation

$$y = x(1+\alpha)/(1+\alpha x/x_c) \tag{3.1}$$

where x is the original expansion variable, y is the new variable, x_c is an estimate of the critical temperature (which need not be particularly accurate, but is a fixed point of the transformation) and α is a user-chosen parameter. As discussed by Nickel (1982), it is important to make α as small as possible, consistent with the desired result that the effect of singularities other than the one of interest be eliminated. The frequent choice $\alpha = 1$ has the disadvantage that the transformed series (in y) effectively utilises only half the original series coefficients (see Guttmann (1989) for an expansion of this point). Thus in this analysis we have chosen α in the range [0.1-0.4], as appropriate. The series thus transformed then have smooth, extrapolable ratios of series coefficients.

Table 3. High temperature series in x for the vacuum energy per site ω_0/N, the susceptibility χ and the mass gap F for the O(3) Heisenberg model. Coefficients of x^n are listed for the line, square and triangular lattices.

n	ω_0/N	χ	F
		Line lattice	
0	0.0	0.333 333 333 3333	2.0
1	0.0	0.222 222 222 2222	−0.666 666 666 666 7
2	−0.083 333 333 333 33	0.094 907 407 4075	0.037 037 037 037
3	0.0	0.032 889 680 4939	0.000 432 098 765 432
4	0.000 057 870 370 37	0.009 930 685 687 35	0.000 327 421 778 039
5	0.0	0.002 574 319 325 70	0.000 020 140 463 593
6	0.000 002 764 366 549	0.000 649 943 687 76	−0.000 016 881 989 548
		Square lattice	
0	0.0	0.333 333 333 333	2.0
1	0.0	0.444 444 444 444	−1.333 333 333 333
2	−0.166 666 666 666 7	0.486 111 111 111	−0.148 148 148 148
3	0.0	0.516 396 604 940	−0.098 353 909 465 0
4	−0.013 194 444 444 4	0.525 667 790 395	−0.024 830 165 262 3
5	0.0	0.528 065 910 445	−0.028 656 708 446
6	−0.002 364 244 929 5	0.522 165 623 325	−0.010 731 673 23
			−0.012 999 698 804 8
		Triangular lattice	
0	0.0	0.333 333 333 333	2.0
1	0.0	0.666 666 666 667	−2.0
2	−0.25	1.173 611 111 111	−0.555 555 555 556
3	−0.083 333 333 333 33	1.955 729 166 667	−0.295 679 012 346
4	−0.041 319 444 444 44	3.166 393 137 31	−0.257 983 049 187
5	−0.026 074 074 074 07	5.035 742 520 30	−0.238 779 221 64
			−0.253 437 328 0

The coefficients of the transformed series were then analysed by the standard ratio method with Neville-Aitken extrapolation; the method of Barber and Hamer (1982), which was designed for the extrapolation of such series; Lubkin's (1952) three-term method, advocated by Drummond (1984) as a powerful general purpose extrapolation scheme; the Bulirsch-Stoer (1964) method, which has been recently applied to such series as ours by Henkel and Schutz (1988); Levin's u transform (Levin 1973); Brezinski's θ transform (Brezinski 1971) and Wynn's ε algorithm (Wynn 1956). These last three have been found by Smith and Ford (1982) to be the most powerful general purpose methods of analysis for logarithmically convergent sequences. These methods are all described, compared and discussed in Guttmann (1989).

In tables 4 and 5 we show a typical analysis of our data—in this case the susceptibility series of the $(2+1)$-dimensional triangular lattice O(2) model. Table 4 shows the result of an inhomogeneous differential approximant analysis (Guttmann 1987a), where we have tabulated the estimates of critical points and critical exponents of $[L/N+\Lambda;\, N]$ approximants, with $\Lambda=-1, 0, 1$. Defective approximants are marked with an asterisk. Combining these following the statistical procedure described in Guttmann (1987a), we obtain the estimate $x_c = 0.2208 \pm 0.0002$, $\gamma = 1.345 \pm 0.025$. In table 5 we show the results of the other seven methods, applied to the extrapolation of the ratio sequence, after the series was first transformed using the transformation (3.1) with $\alpha = 0.1$ and

Table 4. Triangular lattice (2+1)-dimensional, O(2) model susceptibility. Differential approximants $[L/N+\Lambda;\ N]$, $\Lambda=-1, 0, 1$, showing estimates of x_c and γ. Defective approximants are marked with an asterisk.

L	Λ	$N=1$	$N=2$	$N=3$
1	−1		0.214 35	0.220 94
			−1.107	−1.353
	0	0.219 88	0.220 89	0.221 08*
		−1.310	−1.352	−1.368
	1	0.220 61	0.221 04	
		−1.338	−1.364	
2	−1	—	0.220 88	0.221 01*
		—	−1.351	−1.362
	0	0.220 44	0.220 56*	
		−1.328	−1.292	
	1	0.220 90	0.221 07*	
		−1.353	−1.367	
3	−1	—	0.220 98	
		—	−1.358	
	0	0.220 71	0.221 04*	
		−1.340	−1.365	
	1	0.221 00		
		−1.360		
4	−1	—	0.220 47	
		—	−1.318	
	0	0.220 84		
		−1.347		
	1	0.221 77*		
		−1.418		
5	−1	—		
		—		
	0	0.220 63		
		−1.334		

$1/x_c = 4.530$. The simple method of Neville–Aitken extrapolation produced the most regular sequences of estimates. These give for $1/y_c$ the estimate 4.531 ± 0.004, while extrapolation of the sequence of linear intercepts of the ratios (not shown) gave the same estimate of y_c, but with half the error. This result maps to $x_c = 0.2207 \pm 0.0001$ under the inverse of (3.1).

This result is consistent with the estimate from the differential approximants, as well as with that obtained from the other extrapolation techniques, as shown in table 5. Most of the other methods, the results of which are shown in table 5, would, however, have error bars five to ten times as large.

A similar analysis was performed for each series, where in each case we extrapolated not only the sequence of ratios, but also the sequence of linear intercepts of the ratios, given by

$$\zeta_n = nr_n - (n-1)r_{n-1} \tag{3.2}$$

where r_n is the ratio, a_n/a_{n-1}, of successive coefficients of the transformed series.

Table 5. Extrapolations of the sequence of ratios of the coefficients of the O(2) model triangular lattice (2+1)-dimensional susceptibility series. r_n are ratios, $e_n^{(k)}$ are kth-order Neville-Aitken extrapolants, $\zeta_n^{(k)}$ are kth-order extrapolants from Lubkin's transform, $bh_n^{(k)}$ are kth-order extrapolants using the Barber-Hamer method, while $u_n^{(k)}$, $\varepsilon_n^{(k)}$, $\theta_n^{(k)}$ and $B\text{-}S_n^{(k)}$ are kth-order extrapolants using Levin's u transform, Wynn's ε algorithm, Brezinski's θ algorithm and the Bulirsch-Stoer algorithm respectively.

n	r_n	$e_n^{(1)}$	$e_n^{(2)}$	$\zeta_n^{(1)}$	$\zeta_n^{(2)}$	$bh_n^{(1)}$	$bh_n^{(2)}$
1	5.4545						
2	5.2300	5.0055					
3	5.0109	4.5729	4.3565	5.4601		−3.7299	
4	4.8969	4.5546	4.5364	5.0050		4.7728	
5	4.8268	4.5464	4.5341	4.5286	5.4534	4.7151	4.6972
6	4.7792	4.5412	4.5310	4.5176	4.5291	4.6785	4.4971
7	4.7447	4.5377	4.5288	4.5169	4.5168	4.6538	4.5154
8	4.7186	4.5359	4.5305	4.5416	4.5172	4.6375	4.5780

n	$u_n^{(1)}$	$u_n^{(2)}$	$\varepsilon_n^{(1)}$	$\varepsilon_n^{(2)}$	$\theta_n^{(1)}$	$B\text{-}S_n^{(1)}$	$B\text{-}S_n^{(2)}$	$B\text{-}S_n^{(3)}$
1						5.4545		
2						5.2301	4.7229	
3	5.4603		−3.7299			5.0110	4.3130	
4	4.4894		4.7728		5.0050	4.8969	4.3860	4.493
5	4.5092	5.0050	4.7151	4.7266	4.5286	4.8269	4.4236	4.500
6	4.5125	4.5287	4.6786	4.6509	4.5176	4.7793	4.4454	4.502
7	4.5139	4.5176	4.6537	4.6276	4.5169	4.7448	4.5927	4.504
8	4.5223	4.5169	4.6375	4.6194	4.5416	4.7187	4.6984	4.509

Similarly, unbiased estimates of the exponent are given by the sequence with terms γ_n, where

$$\gamma_n = [n(2-n)r_n + (n-1)^2 r_{n-1}]/\zeta_n. \tag{3.3}$$

Once x_c has been estimated, *biased* exponent estimates can be obtained from the sequence $\{\gamma_n^b\}$, with elements

$$\gamma_n^b = (n x_c r_n - n + 1). \tag{3.4}$$

Both the biased and unbiased exponent sequences were also extrapolated by all seven sequence extrapolation algorithms for all series.

The results of this analysis is summarised in table 6 for the (2+1)-dimensional susceptibility series and mass gap series, which give estimates of the exponents γ and ν respectively. We have not analysed the series for the vacuum energy, as they are rather shorter than the other series, and also more difficult to analyse. For the line lattice, our analysis of the O(2) model gave an estimate of $x_c = 1.55 \pm 0.20$, but no value of the critical exponent consistent with a conventional algebraic singularity was found. A subsequent analysis that assumed a Kosterlitz-Thouless-type singularity indicated that the series were too short for confident assertions about the nature of the singularity from these series alone. Another analysis of these series, and other data pertaining to this problem, is to be found in Allton and Hamer (1988). For the O(3) model on the line lattice we found no evidence of a critical point.

A comparison of our analysis with previous analyses is given in table 7 for the Ising model. For comparison we also give the results of a representative analysis of

Table 6. Summary of results of analyses described in text for (2 + 1)-dimensional susceptibility series and mass gap series. The confidence limits are shown bracketed after each entry.

Model	x_c	γ (unbiased)	γ (biased)	ν (unbiased)	ν (biased)
		Square lattice			
Ising	0.328 5 (4)	1.239 (5)	1.245 (4)	0.646 (8)	0.640 (5)
O(2)	0.348 0 (10)	1.33 (3)	1.310 (5)	0.695 (4)	0.676 (10)
O(3)	1.080 (5)	1.41 (4)	1.40 (1)	0.724 (8)	0.724 (4)
		Triangular lattice			
Ising	0.209 72 (7)	1.234 (4)	1.242 (2)	0.646 (8)	0.640 (5)
O(2)	0.220 7 (1)	1.33 (1)	1.334 (5)	0.686 (3)	0.686 (3)
O(3)	0.678 3 (4)	1.397 (1)	1.395 (5)	0.713 (5)	0.713 (2)

Table 7. A comparison of previous calculations with results obtained in this work for the (2+1)-dimensional Ising model: HTFT = High-temperature field theory, LTFT = Low-temperature field theory, FSS = Finite-size scaling, EL = Euclidean lattice model.

Calculation	ν	γ	x_c
	Square lattice		
HTFT Hamer and Irving 1984	0.66 (2)	1.257 (10)	0.329 0 (10)
LTFT Marland 1981	—	$\gamma' = 1.25$	0.329 (1)
FSS Hamer 1983	0.635 (5)	—	0.329 (1)
FSS Henkel 1984	0.629 (2)	—	0.328 (1)
This work	0.646 (8) ub	1.239 (5) ub	0.328 5 (4)
	0.640 (5) b	1.245 (4) b	
EL Guttmann 1987b	0.632 (3)	1.239 (3)	N.A.
	Triangular lattice		
HTFT Hamer and Irving 1984	0.64 (2)	1.247 (5)	0.209 76 (15)
LTFT Marland 1981	—	$\gamma' = 1.250$ (12)	0.209 8 (2)
FSS Hamer and Johnson 1986	0.627 (4)	1.236 (8)	0.209 6 (2)
This work	0.646 (8) ub	1.243 (4) ub	0.209 72 (7)
	0.640 (5) b	1.242 (2) b	
EL Guttmann 1987b	0.632 (3)	1.239 (3)	N.A.

the Euclidean lattice spin model. It can be seen that the analysis of the mass-gap series presented here is less accurate than analyses based on finite-size scaling (Hamer 1983, Henkel 1984, Hamer and Johnson 1986), while the analysis of the susceptibility series is significantly more accurate than any previous analysis, as is the estimate of the critical point. Comparison with recent series estimates (Guttmann 1987b) demonstrates satisfying consistency between the Euclidean lattice model and its counterpart in Hamiltonian lattice field theory.

4. Conclusions

Our final estimates for the critical parameters of the three models on the square and triangular lattices are summarised in table 6. These are the first accurate estimates which have been made for the O(2) and O(3) Heisenberg models.

For the Ising model, earlier series estimates have been given by Marland (1981) and by Hamer and Irving (1984). Our results are generally in good agreement with those earlier estimates, but are about twice as accurate. Finite-size scaling analyses have also been made by Hamer (1983) and Henkel (1984) for the square lattice, and by Hamer and Johnson (1986) for the triangular lattice. For the critical index ν, in particular, they obtained results 0.635 (5), 0.629 (2) and 0.627 (4) respectively which are slightly lower and perhaps slightly more accurate than ours.

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