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The Ising model with a free surface: a series analysis study

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Abstract. We have generated series expansions for the layer susceptibility χ_1 of the Ising model with a free surface, on both the square and simple cubic lattices. In both cases we have extended known series expansions by four terms. Analysis of these series yields $\gamma_1 = 1{\cdot}37 \pm 0{\cdot}01$ (square) and $\gamma_1 = 0{\cdot}78 \pm 0{\cdot}02$ (simple cubic). These results are consistent with both surface scaling and with the recent RG scaling result obtained by A J Bray and M A Moore.

1. Introduction

The behaviour of magnetic systems with a free surface has been the subject of several recent studies. The position up to 1976 is discussed by Binder and Landau (1976), but since that time there have been several relevant RG calculations (Lubensky and Rubin 1975, Svrakić and Wortis 1977, Burkhardt and Eisenriegler 1977, Bray and Moore 1977) and a series analysis study of the self-avoiding walk problem (Barber *et al* 1978). As pointed out by Binder and Landau (1976), this problem is of interest, not only because of its theoretical significance, but also for its applicability to catalysis phenomena. This is particularly relevant to the current problem as the magnetic properties of catalyst surfaces are believed to be related to their catalytic properties.

The model we have studied is described by the Hamiltonian

$$\mathscr{H} = -J \sum_{\langle ij \rangle} \mu_i \,.\, \mu_j - mH \sum_i \mu_i - mH_l \sum_i{}' \mu_i. \tag{1.1}$$

This is the usual Ising spin Hamiltonian with the addition of a surface magnetic field H_l, which is parallel to the bulk magnetic field H_l but acts only on the surface spins, as implied by the prime on the summation.

The surface magnetic field allows the definition of two additional susceptibilities; the layer susceptibility χ_1 given by $-\partial^2 G/\partial H\, \partial H_1$, where G is the Gibbs free energy, and the local susceptibility χ_{11} given by $-\partial^2 G/\partial H_1^2$, in addition to the bulk susceptibility $\chi = -\partial^2 G/\partial H^2$. For these two additional susceptibilities we define corresponding exponents γ_1 and γ_{11} respectively, i.e. $\chi_1 \sim (T-T_c)^{-\gamma_1}$ and $\chi_{11} \sim (T-T_c)^{-\gamma_{11}}$ as $T \to T_c^+$. We also assert that the critical temperature for these additional susceptibilities is the same as for the bulk system. In two dimensions this follows from the exact result of McCoy and Wu (1975), which establishes that χ and χ_{11} have the same critical temperature. Given the nature of the graphical expansion of the different susceptibilities (as

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discussed in the next section), we can bound the series coefficients in the high-temperature expansion of χ_1 both above and below by those of χ and χ_{11}, from which follows the identity of their radii of convergence, and hence their critical temperatures. In three dimensions we have no explicit proof, but such a result is most unlikely to be dimension-dependent, and has in any event been proved for the $d=3$, $n=0$ case (Whittington 1975) so that we feel confident in assuming it here.

The above critical exponents are not independent, but are expected to be related through the surface scaling relation (Barber 1973) $2\gamma_1 - \gamma_{11} = \gamma + \nu$. One of our aims is to test the validity of this relation, which we found to be satisfied for the $n=0$ problem (Barber *et al* 1978). Another aim is to test the less-well founded RG scaling relation of Bray and Moore (1977): $\gamma_{11} = \nu - 1$. This important relation was found not to be satisfied for the two-dimensional $n=0$ model, and was only just within fairly wide confidence limits for the three-dimensional $n=0$ model (Barber *et al* 1978). However, for the two-dimensional Ising model it is clearly satisfied as $\gamma_{11}=0$ and $\nu=1$ (McCoy and Wu 1973). For the Ising model in three dimensions it is therefore of considerable interest to test its validity.

We have therefore generated series expansions for χ_1 on both the square and simple cubic lattices, obtaining 14 and 12 coefficients respectively on the two lattices. In an earlier study, Binder and Hohenberg (1972, 1974) obtained 10 and 8 coefficients for this quantity on the same lattices. Binder and Hohenberg also studied a wide range of transitions obtainable by varying the ratio of the coupling constant in the surface to that in the bulk. We have not considered that aspect here.

In the next section we shall describe the derivation of the series. In § 3 we present an analysis of the series. The final section comprises a discussion of our results.

2. Derivation of the series

For the bulk Ising model, a variety of methods for deriving series expansions of the susceptibility exists. The earliest of these methods, and the most obvious, is due to Oguchi (1949). In that method one requires all graphs with two odd vertices embeddable in the underlying lattice, with the constraint that multiple occupancy of a bond is forbidden. The disadvantage of the method is that a large number of graphs is required, including multicomponent graphs. Several methods exist which reduce the number of graphs; one of these methods requires only connected graphs, while the star graph method requires only connected graphs with no cut points (see Domb 1974 for a review). Unfortunately the implementation of those methods which make use only of connected graphs depends on the translation invariance of the lattice, a feature which is manifestly absent in the present problem. While these methods could presumably be appropriately modified to handle this feature, we decided to use the original (Oguchi 1949) method, which is directly applicable. Furthermore, a list of the required topologies was already available (Guttmann and Nymeyer 1977) for all graphs up to 12 lines on the square and simple cubic lattices.

In accordance with previous studies (Binder and Hohenberg 1972, 1974) we chose the square and simple cubic lattices. It may also be argued that these lattices are the most natural choice if one requires a rectilinear boundary.

The graphs required for the layer susceptibility χ_1 are all graphs with two odd vertices, with the constraints that at least one odd vertex lies in the surface and no vertices lie below the surface. The subset of these graphs, comprising the set of graphs with both odd vertices in the surface, is required to generate the series expansion for the local susceptibility χ_{11}. We deliberately chose not to extend this series for several reasons. Firstly, for the square lattice the corresponding exponent γ_{11} is known exactly (McCoy and Wu 1973), so there is little purpose in studying this quantity by series analysis. Secondly, our graph counting programs do not automatically produce the required breakdown into layer and local susceptibility graphs, though this objection could be overcome. The third and most compelling reason is that we consider that the extension of this series for the simple cubic lattice would avail us very little. The expected critical exponent γ_{11} is small and negative. Such exponents are notoriously difficult to analyse (Gaunt and Guttmann 1974). Our experience with the self-avoiding walk analogue of this problem (Barber *et al* 1978) leads us to believe that a series longer than that which we could derive here would be needed to give a reliable estimate of γ_{11}. For the self-avoiding walk problem our series for χ_{11} was 23 terms long for the square lattice and 14 terms long for the simple cubic lattice. For the Ising problem our series are 14 and 12 terms long respectively for the two lattices.

We therefore required graphs with up to four components. (A four-component graph first becomes embeddable on these lattices at 13 lines, while five-component graphs do not occur before 17 lines.) The one-component graphs were counted using a modified version of the counting program written by J L Martin and C J Elliott. New programs were written to count the two-component graphs. The symbolic counting methods developed by M F Sykes (1979 private communication) were used to express the three- and four-component graphs in terms of two-component graphs, which could then be counted by machine.

Most disconnected graphs were also checked by hand calculations. All calculations and the tabulation and consolidation of individual results were performed independently by at least two of us, and usually by all three of us. We therefore have a high degree of confidence in the accuracy of our series coefficients.

The layer susceptibility series has thus been extended by four terms on both the square and simple cubic lattices. Since these coefficients grow exponentially, such an extension is substantial. We list the coefficients in table 1 below. The first 8 coefficients

Table 1. Coefficients of the layer susceptibility χ_1 for the square and simple cubic lattices.

n	χ_1 (square)	χ_1 (simple cubic)
0	1	1
1	3	5
2	7	21
3	19	93
4	49	409
5	127	1837
6	321	8209
7	813	36969
8	2041	166041
9	5117	748889
10	12763	3373941
11	31791	15248153
12	78917	68840633
13	195677	
14	484019	

for the simple cubic lattice and the first 10 coefficients for the square lattice were previously obtained by Binder and Hohenberg (1972, 1974) and we are happy to report complete agreement with their coefficients as published in 1974.

3. Analysis of series

As discussed in § 1 the critical point for the layer susceptibility χ_1 is expected to be the same as for the bulk. Utilising this fact, our analysis methods are all biased by specifying the critical temperature. This is exactly known for $d=2$ ($V_c^{-1}=1+\sqrt{2}$), while for $d=3$ the series estimate $V_c^{-1}=4\cdot5844$ (Sykes *et al* 1972) is expected to be uncertain only in the last digit.

We have analysed the series for the exponent γ_1 using standard ratio techniques modified to take into account the oscillations in the ratio plots characteristic of a loose-packed lattice (Gaunt and Guttmann 1974). If the ratio of alternate coefficients a_n/a_{n-2} is denoted r_n, then estimates of the exponent are given by the sequence $\gamma_1^{(0)}(n)=\frac{1}{2}n(V_c^2r_n-1)+1$. Linear extrapolants of alternate terms, given by

$$\gamma_1^{(1)}(n)=\tfrac{1}{2}[n\gamma_1^{(0)}(n)-(n-2)\gamma_1^{(0)}(n-2)]$$

take account both of a period two oscillation in the ratio plots, and of a correction term $O(n^{-2})$ in the ratios. Higher-order extrapolants may also be defined if the regularity of the series warrants such a refinement.

For the square and simple cubic lattices, we show these extrapolations in table 2. For the square lattice, the exponent estimates slowly increase and suggest a value $\gamma_1 \geqslant 1\cdot366$, while the linear extrapolants are slightly higher, though more erratic, and suggest a value $\gamma_1 \sim 1\cdot372$. Taking this as our central value, we estimate a confidence limit that takes into account the last five entries in the table as well as discernible trends, and we thus give as our final estimate $\gamma_1=1\cdot372\pm0\cdot01$.

For the simple cubic lattice the exponent estimates are decreasing quite rapidly, giving $\gamma_1<0\cdot825$, while the last five entries of the linear extrapolants are quite stable

Table 2. Ratios and extrapolants to estimate the layer susceptibility exponent γ_1 for the square and simple cubic lattices.

	Square lattice			Simple cubic lattice		
n	a_n/a_{n-2}	$\gamma_n^{(0)}$	$\gamma_n^{(1)}$	a_n/a_{n-2}	$\gamma_n^{(0)}$	$\gamma_n^{(1)}$
3	6·333333	1·1300	—	18·600000	0·8275	—
4	7·000000	1·4020	—	19·476190	0·8534	—
5	6·684211	1·3671	1·7228	19·752688	0·8496	0·8828
6	6·551020	1·3720	1·3118	20·070905	0·8650	0·8882
7	6·401575	1·3442	1·2870	20·124660	0·8514	0·8560
8	6·358255	1·3637	1·3388	20·226702	0·8496	0·8036
9	6·293973	1·3595	1·4129	20·257216	0·8374	0·7882
10	6·253307	1·3646	1·3681	20·319927	0·8342	0·7726
11	6·212820	1·3628	1·3777	20·361032	0·8284	0·7880
12	6·183264	1·3654	1·3694	20·403627	0·8250	0·7787
13	6·155107	1·3644	1·3732			
14	6·133267	1·3662	1·3713			

and suggest a value around 0·78. Estimating the confidence limits in a similar manner to that employed for the square lattice leads to the final estimate $\gamma_1 = 0{\cdot}78 \pm 0{\cdot}02$. Varying the critical point estimates by one part in 10^4 did not change these estimates at all.

Other methods of analysis have also been employed. In order to remove the oscillation of the ratio plots, we transformed the series using the Euler transformation

$$X = 2V/(1 + V/V_c).$$

This transformation leaves the origin and the point $V = V_c$ invariant, while moving the point $V = -V_c$ to infinity in the X plane. The transformed series were then analysed by standard ratio techniques, including Neville table extrapolations. The results, though not shown here, are entirely consistent with those quoted above.

4. Discussion

In Barber *et al* (1978) we studied the corresponding susceptibilities for the self-avoiding walk problem, and found that the surface scaling relation (Barber 1973) $2\gamma_1 - \gamma_{11} = \gamma + \nu$ was satisfied, while the RG scaling relation (Bray and Moore 1977) $\gamma_{11} = \nu - 1$ was not satisfied for the two-dimensional system.

For the Ising problem, it is known that the RG scaling relation $\gamma_{11} = \nu - 1$ is satisfied for the two-dimensional system, since the exact results $\gamma_{11} = 0$, $\nu = 1$ are known (McCoy and Wu 1973). Combining these results with the exact result $\gamma = \frac{7}{4}$ gives the surface scaling prediction $\gamma_1 = 1{\cdot}375$. Our series result $\gamma_1 = 1{\cdot}372 \pm 0{\cdot}01$ is in excellent agreement with this, and so provides additional support, if any were needed, for the validity of surface scaling for this system.

For the three-dimensional system there are of course no relevant exact results. The best series estimates for the bulk quantities are $\gamma = 1{\cdot}250 \pm 0{\cdot}003$ and $\nu = 0{\cdot}638^{+0{\cdot}002}_{-0{\cdot}001}$ (Ferer and Wortis 1972). Surface scaling therefore gives $2\gamma_1 - \gamma_{11} = 1{\cdot}888^{+0{\cdot}005}_{-0{\cdot}004}$, while the RG scaling relation gives $\gamma_{11} = -0{\cdot}362^{+0{\cdot}001}_{-0{\cdot}002}$. As discussed in § 2, we have not attempted to obtain series estimates of γ_{11}, and so we cannot test surface scaling directly. However, since surface scaling appears to hold for the self-avoiding walk problem in both two and three dimensions, as well as the Ising model in two dimensions and for all other systems for which it has been tested, it seems reasonable to assume its validity for the three-dimensional Ising model. Accepting this, our series estimate $\gamma_1 = 0{\cdot}78 \pm 0{\cdot}02$, when combined with surface scaling, gives $\gamma_{11} = -0{\cdot}33 \pm 0{\cdot}04$. The confidence limits are sufficiently wide to include readily the RG scaling result, and so our result is entirely consistent with the RG scaling result of Bray and Moore (1977), though not perhaps with a level of precision that would be conclusive. This is in contrast to the earlier result of Binder and Hohenberg (1972) who obtained $\gamma_1 \sim 0{\cdot}88$, which when combined with surface scaling gave $\gamma_{11} = -0{\cdot}13$. However, this result is clearly a consequence of the extrapolation of a series that is too short, a fact that was recognised by Binder and Hohenberg at the time. Indeed the ratio plots for the γ_1 series for the simple cubic lattice exhibit considerable curvature, and the additional four terms we obtained were vital in determining the exponent. A careful study of our results suggest that an additional six series coefficients would be required to obtain a level of precision in the estimate of γ_1 that would be conclusive. That is not a practical procedure employing the methods used here, but may be possible using an appropriately modified version of the star graph method.

An alternative procedure that tests the combination of surface scaling with RG scaling has also been employed. Combining the surface scaling relation $2\gamma_1 - \gamma_{11} = \gamma + \nu$ with the RG scaling result $\gamma_{11} = \nu - 1$ gives $2\gamma_1 - 2\nu - \gamma + 1 = 0$. The surface susceptibility coefficients

$$a_n \sim A\mu^n n^{\gamma_1 - 1},$$

while the series coefficients of the second spherical moment (Moore *et al* 1969) $b_n \sim B\mu^n n^{-\gamma-2\nu-1}$. It follows therefore that the sequence $\{e_n\}$, whose elements are defined by $e_n = n^2 a_n^2 / b_n \mu^n$, behaves asymptotically as n^ϕ, where $\phi = 2\gamma_1 - 2\nu - \gamma + 1$. This result holds irrespective of the value of the individual exponents γ_1, ν and γ. If the combination of surface scaling and RG scaling is correct, the exponent ϕ should be zero. For the simple cubic lattice we have estimated ϕ by forming the sequences $\{\phi_n^{(0)}\}$ and $\{\phi_n^{(1)}\}$, defined by

$$\phi_n^{(0)} = \tfrac{1}{2}n(e_n/e_{n-2} - 1); \qquad \phi_n^{(1)} = \tfrac{1}{2}[n\phi_n^{(0)} - (n-2)\phi_{n-2}^{(0)}]. \tag{4.1}$$

These sequences are shown in table 3. It can be seen that the sequence $\{\phi_n^{(0)}\}$ is decreasing rapidly, while the linear extrapolants $\{\phi_n^{(1)}\}$ are sporadically oscillating around a value of zero. The estimate $|\phi| < 0.03$ contains four of the last five estimates, and provides additional support for our earlier conclusions with a similar level of precision.

Table 3. Direct test of surface scaling and RG scaling for the simple cubic lattice.

n	e_n	$\phi_n^{(0)}$	$\phi_n^{(1)}$
5	1·631139	0·8752	−0·1850
6	1·708034	0·8192	0·1440
7	1·787323	0·6703	0·1579
8	1·837954	0·6085	−0·0235
9	1·889529	0·5147	−0·0300
10	1·924837	0·4727	−0·0705
11	1·962558	0·4251	0·0224
12	1·987900	0·3931	−0·0047

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References

Barber M N 1973 *Phys. Rev.* **B8** 407–9

Barber M N, Guttmann A J, Middlemiss K M, Torrie G M and Whittington S G 1978 *J. Phys. A: Math. Gen.* **11** 1833–42

Binder K and Hohenberg P C 1972 *Phys. Rev.* **B6** 3461–87

—— 1974 *Phys. Rev.* **B9** 2194–214

Binder K and Landau D P 1976 *Surf. Sci.* **61** 577–602

Bray A J and Moore M A 1977 *J. Phys. A: Math. Gen.* **10** 1927–62
Burkhardt T W and Eisenriegler E 1977 *Phys. Rev.* B**16** 3213–21
Domb C 1974 *Phase Transitions and Critical Phenomena*, vol. 3 ed C Domb and M S Green (London: Academic Press)
Ferer M and Wortis M 1972 *Phys. Rev.* B **6** 3426–44
Gaunt D S and Guttmann A J 1974 *Phase Transitions and Critical Phenomena* vol. 3 ed C Domb and M S Green (London: Academic Press)
Guttmann A J and Nymeyer A 1977 *Research Report* Department of Mathematics, University of Newcastle p 188
Lubensky T C and Rubin M H 1975 *Phys. Rev.* B**11** 4533–46
McCoy B M and Wu T T 1973 *The Two Dimensional Ising Model* (Cambridge, Mass.: Harvard University Press)
Moore M A, Jasnow D and Wortis M 1969 *Phys. Rev. Letts.* **22** 940–3
Oguchi T 1949 *Phys. Rev.* **76** 1001
Svrakić N M and Wortis M 1977 *Phys. Rev.* B **15** 396–402
Sykes M F, Gaunt D S, Roberts P D and Wyles J A 1972 *J. Phys. A*: *Math. Gen.* **5** 640
Whittington S G 1975 *J. Chem. Phys.* **63** 779