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The square lattice Ising model with a free surface

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Abstract. Using the appropriately generalised finite lattice method, series expansions of the layer (χ_1) and local (χ_{11}) susceptibilities of the square lattice Ising model have been obtained. They extend existing series by 3 and 13 terms for χ_1 and χ_{11}, respectively. Series analysis yields the exponent estimates $\gamma_1 = 1{\cdot}375 \pm 0{\cdot}005$ and $\gamma_{11} = 0{\cdot}00 \pm 0{\cdot}01$, in agreement with scaling predictions. Repetition of the analysis used in the analogous self-avoiding walk problem confirms the breakdown of the renormalisation group scaling relation $\gamma_{11} = \nu - 1$ for the square lattice self-avoiding walk problem found in an earlier study.

1. Introduction

In this paper the finite lattice method (de Neef 1975) has been used to extend series expansions for the reduced, isothermal, layer susceptibility χ_1 and reduced, isothermal, local susceptibility χ_{11} of the square lattice Ising model. The model is described by the Hamiltonian

$$\mathscr{H} = -J \sum_{\langle ij \rangle} \mu_i \mu_j - mH \sum_i \mu_i - mH_1 \sum_i{}' \mu_i. \tag{1.1}$$

This is the usual Ising spin Hamiltonian with the addition of a surface magnetic field H_1, which is parallel to the bulk magnetic field H 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 reduced isothermal layer susceptibility χ_1 where $\beta m^2 \chi_1 = (-\partial^2 G/\partial H \partial H_1)$ where G is the Gibbs free energy, and the reduced isothermal local susceptibility χ_{11}, where $\beta m^2 \chi_{11} = -\partial^2 G/\partial H_1^2$, 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, that is, $\chi_1 \sim (T - T_c)^{-\gamma_1}$ and $\chi_{11} \sim (T - T_c)^{-\gamma_{11}}$ as $T \to T_{c^+}$, where $\tanh(J/kT_c) = \sqrt{2} - 1$, as in the bulk case (McCoy and Wu 1973).

The finite lattice method for obtaining high-temperature series expansions for model systems on the square lattice was obtained by de Neef (1975) using heuristic arguments. The first description of the combinatorial enumeration implicit in the method was given by de Neef and Enting (1977) although some of the relevant results go back to the work of Hijmans and de Boer (1955). An alternative form of the finite lattice method was described by Enting and Baxter (1977), and Enting (1978a) has constructed generalised Möbius functions to describe the combinatorial factors which

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are common to the two forms of the finite lattice method. The formalism has subsequently been extended to include low-temperature expansions (Enting 1978b).

In the finite lattice method, series expansions are obtained by combining the partition functions or free energies of various finite rectangular sublattices of the infinite square lattice. The formal description below is based on using a sum of free energies. It is usually convenient to modify the formalism to work with reduced free energies. This is essentially a matter of ignoring the various trivial factors such as ln cosh βJ. The other main modification is to exponentiate the expressions for the (reduced) free energy as a linear combination of (reduced) free energies for finite lattices, thus obtaining the (reduced) partition function series as a product of powers of finite lattice (reduced) partition functions. Working with products of partition functions usually provides the computationally desirable feature that only integers are needed in the calculations.

Using the finite lattice method we have extended the recently obtained series expansion of χ_1 (Whittington *et al* 1979a) from 14 to 17 terms, and have extended the expansion of χ_{11} (Binder and Hohenberg 1972) from 10 to 23 terms.

These extended series allow us to estimate the exponent γ_1 with greater precision than heretofore, and we obtained the estimate $\gamma_1 = 1{\cdot}375 \pm 0{\cdot}005$, in precise agreement with the scaling prediction $\gamma = 1\frac{3}{8}$. For the local susceptibility χ_{11}, McCoy and Wu (1973) have obtained the exact result $\gamma_{11} = 0$, corresponding to a logarithmic divergence. While there is therefore little to be gained by a *series* estimate of γ_{11}, this series expansion is of considerable utility in testing the method of analysis used by Barber *et al* (1978) in their analysis of some surface scaling properties of the self-avoiding walk (SAW) analogues of χ_1 and χ_{11}. In Barber *et al* (1978) the surface scaling relation $2\gamma_1 - \gamma_{11} = \gamma + \nu$ (Barber 1973) and the renormalisation group (RG) scaling relation $\gamma_{11} = \nu - 1$ (Bray and Moore 1977) were tested by a variety of methods of series analysis for the square and simple cubic lattice SAW models. For the square lattice Ising model both these relations are satisfied (Whittington *et al* 1979a), but for the SAW model on the square lattice it was found that, while surface scaling appears to hold, the RG scaling relation failed by an amount $\theta = 0{\cdot}05 \pm 0{\cdot}01$, where $\theta = \gamma_{11} - \nu + 1$.

In this paper we have employed the same method of analysis as Barber *et al* (1978) but applied it to the analogous square lattice Ising series. For χ_{11} the Ising and SAW series were of identical length (23 terms) while for χ_1 the Ising series is of length 17 terms compared to 21 for the SAW series.

Our Ising series analysis clearly indicates the validity of both surface scaling and RG scaling, thus strengthening considerably the earlier conclusions of Barber *et al* (1978) that RG scaling fails for the square lattice SAW model.

In the next section we describe the derivation of the series expansions by the finite lattice method, and in § 3 we perform the analysis. Section 4 consists of a summary and discussion.

2. Series derivation

The finite lattice method starts from the general form of series expansions for the free energy on a graph g as a sum of cluster weights,

$$f(g) = \sum_{g' \leq g} h(g')t(g', g) \tag{2.1}$$

where $t(g', g)$ is the number of ways g' can be embedded in g.

The finite lattice method is useful in the case where
(i) $h(g')$ is zero if g' is disconnected, and
(ii) $h(g')$ can be used as the basis for a series expansion.
That is, for any finite power of the expansion variable, only a finite number of graphs contribute.

In these circumstances, (2.1) can be resummed for square lattice systems to give an expression of the same form but involving only rectangular graphs:

$$f[m, n] = \sum_{i=1}^{m} \sum_{j=1}^{n} h[i, j] t([i, j], [m, n]) \tag{2.2}$$

where

$$\begin{aligned} t([i, j], [m, n]) &= (m-i+1)(n-j+1) \qquad && 1 \leq m, j \leq n \\ &= 0 && \text{otherwise.} \end{aligned} \tag{2.3}$$

The $[i, j]$ denote rectangles of i sites by j sites. Equation (2.2) can be inverted to give

$$h[m, n] = \sum_{i} \sum_{j} f[i, j] \nu([i, j], [m, n]) \tag{2.4a}$$

where

$$\nu([i, j], [m, n]) = \eta(i, m) \eta(j, n) \tag{2.4b}$$

and

$$\begin{aligned} \eta(i, m) &= 1 \qquad && i = m \text{ or } i+2 = m \\ &= -2 && i+1 = m \\ &= 0 && \text{otherwise.} \end{aligned} \tag{2.4c}$$

For large lattices we let $m, n \to \infty$ and find 'bulk' free energies from

$$\lim_{M,N \to \infty} f[m, n]/mn \to \sum_{i,j} h[i, j]. \tag{2.5}$$

Similarly Enting (1978a) has shown how certain surface contributions can be obtained by extracting terms proportional to m or n as $m, n \to \infty$.

To obtain more general surface properties such as surface susceptibilities the boundaries have to be considered explicitly as having interactions different from those in the bulk. The simplest arrangement is shown in figure 1. We must consider factors

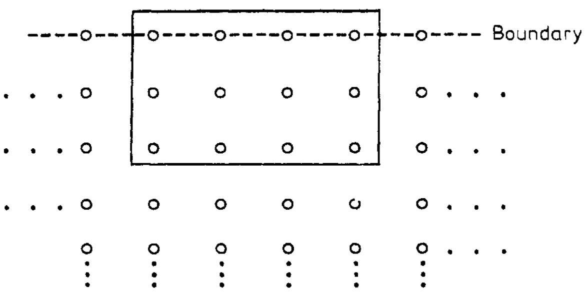

Figure 1. A typical graph required to calculate surface properties, in this case $f^*[4, 3]$.

$f^*[m,n]$, $h^*[m,n]$ for sublattices with one edge lying on the boundary. In this case (2.2) becomes

$$f^*[m,n]=\sum_{i\leq m}\sum_{j\leq n}(m-i+1)\{h^*[i,j]+(n-j)h[i,j]\}.$$

Defining

$$\begin{aligned} t^*([i,j],[m,n]) &= (m-i+1) \qquad && m\geq i \quad n\geq j \\ &= 0 && \text{otherwise,} \end{aligned}$$

its inverse is

$$\nu^*([i,j],[m,n])=\eta(i,m)\xi(j,n)$$

where

$$\begin{aligned} \xi(j,n) &= 1 \qquad && j=n \\ &= -1 && j+1=n \\ &= 0 && \text{otherwise.} \end{aligned}$$

If $x=\tanh\beta H_1$ and $y=\tanh\beta H$ then $(\chi_{11}-1)/2$ is the coefficient of x^2 in the free energy expansion, and $\chi_1-\chi_{11}$ is the coefficient of xy.

None of the $h[i,j]$ involves x so that χ_1, χ_{11} can be obtained from sums of $h^*[i,j]$ alone.

The use of connected graph expansion formalisms for susceptibility is based on the formalism of Domb (1972, § 6). This formalism helps determine the cut-off of the expansion. Expanding in powers of $v=\tanh\beta J$ the contribution of $h^*[i,j]$ to χ_{11} is at least of order v^{i+2j-3} while the contribution to χ_1 is at least of order v^{i+j-2}.

Since the finite lattice free energies are obtained using transfer matrix methods, the natural cut-off for the expansion is in terms of a maximum 'width' of rectangle. This width may be chosen to be either parallel or perpendicular to the boundary.

For matrices of dimension 2^k we can evaluate $h^*[i,j]$ for all i, j such that $i\leq k$ or $j\leq k$. This means that χ_{11} is correct to v^{3k-1} and χ_1 is correct to v^{2k-1} (inclusive).

For χ_{11} we use the sum $\Sigma_{i=1}^{3k}\Sigma_{j=1}^{3k+2-i}h^*[i,j]$ and extract the coefficient of x^2, while for χ_1 we form the sum $\Sigma_{i=1}^{2k}\Sigma_{j=1}^{2k+1-i}h^*[i,j]$ and extract the coefficient of xy, where in both cases

$$h^*[i,j]=\sum_{p\leq i}\sum_{q\leq j}\nu^*([p,q],[i,j])\{f^*[p,q]-\sum_{m\leq p}{}'\sum_{n\leq q}{}'(p-m+1)(q-n)h[m,n]\}.$$

Since $h[m,n]$ is of order $v^{2(m+n-2)}$ the primed summations can be truncated at the appropriate limit for the particular calculation.

In this way we have obtained 17 terms in the expansion of $\chi_1=\Sigma_{n\geq0}c_n^{(1)}v^n$, where $v=\tanh(J/kT)$, and 23 terms in the expansion of $\chi_{11}=\Sigma_{n\geq0}c_n^{(1,1)}v^n$, and these are shown in table 1. They confirm the earlier work of Whittington *et al* (1979a) and indicate a typographical error in the coefficient of v^{10} in the series for χ_{11} given by Binder and Hohenberg (1972).

3. Series analysis

We first attempt to form direct estimates of γ_1 and γ_{11}. Because of the odd–even alternation in the ratios we have used the Euler transformation $z=2v(1+v/v_c)^{-1}$ to

Table 1. Coefficients of the layer and local susceptibilities, χ_1 and χ_{11}.

n	Layer susceptibility $c_n^{(1)}$	Local susceptibility $c_n^{(1,1)}$
0	1	1
1	3	2
2	7	2
3	19	4
4	49	8
5	127	18
6	321	36
7	813	80
8	2041	170
9	5117	382
10	12 763	832
11	31 791	1884
12	78 917	4178
13	195 677	9526
14	483 997	21 388
15	1196 081	49 040
16	2950 439	111 130
17	7271 905	256 002
18		584 290
19		1351 284
20		3101 736
21		7197 354
22		16 597 682
23		38 624 304

map the singularity at $v = -v_c$ in the susceptibilities to infinity, leaving the physical singularity at $v = v_c$ unchanged. Using the exact value of $v_c = \sqrt{2}-1$ we have formed ratio estimates, such as

$$\gamma_{1,n} - 1 = n[(c_n^{(1)} v_c / c_{n-1}^{(1)}) - 1], \tag{3.1}$$

and extrapolated these using standard Neville table methods (see, for example, Gaunt and Guttmann 1974). Results for γ_1 for the square lattice are given in table 2. These suggest

$$\gamma_1 = 1{\cdot}372 \pm 0{\cdot}008. \tag{3.2}$$

We have also analysed the untransformed series, 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 $\gamma_1^{(0)}(n) = \frac{1}{2}n(v_c^2 r_n - 1) + 1$. Linear extrapolants of alternate terms, given by $\gamma_1^{(1)}(n) = \frac{1}{2}[n\gamma_1^{(0)}(n) - (n-2)\gamma_1^{(0)}(n-2)]$, take account of both a period 2 oscillation in the ratio plots, and a correction term $O(1/n^2)$ in the ratios. Higher order extrapolants may also be defined if the regularity of the series warrants such a refinement. The results of this analysis are shown in the last two columns of table 2, and allow us to make the final estimate $\gamma_1 = 1{\cdot}375 \pm 0{\cdot}005$.

For γ_{11} on the square lattice, the results of a ratio analysis on the transformed series are given in table 3. The linear extrapolants suggest that $\gamma_{11} < 0{\cdot}027$ and the quadratic

Table 2. Ratio estimates of γ_1 for the square lattice. α_n are ratio estimates from the transformed series, and $\alpha_n^{(1)}$ and $\alpha_n^{(2)}$ are the linear and quadratic extrapolants of the sequence $\{\alpha_n\}$. $\gamma_n^{(0)}$ and $\gamma_n^{(1)}$ are estimates based on alternate ratios of the untransformed series.

n	α_n	$\alpha_n^{(1)}$	$\alpha_n^{(2)}$	$\gamma_n^{(0)}$	$\gamma_n^{(1)}$
8	1·2600	1·3583	1·3058	1·3637	1·3388
9	1·2697	1·3468	1·3065	1·3595	1·4129
10	1·2769	1·3423	1·3242	1·3646	1·3681
11	1·2829	1·3430	1·3464	1·3628	1·3777
12	1·2883	1·3467	1·3649	1·3654	1·3694
13	1·2931	1·3513	1·3768	1·3644	1·3732
14	1·2976	1·3558	1·3824	1·3662	1·3713
15	1·3017	1·3594	1·3833	1·3656	1·3737
16	1·3055	1·3622	1·3815	1·3669	1·3721
17	1·3089	1·3641	1·3787	1·3666	1·3739

Table 3. Ratio estimates of γ_{11} for the square lattice. α_n are ratio estimates from the transformed series and $\alpha_n^{(1)}$ and $\alpha_n^{(2)}$ are the linear and quadratic extrapolants of the sequence $\{\alpha_n\}$. ϵ_n are the averages of successive exponent estimates obtained from linear extrapolants of alternate exponent estimates.

n	α_n	$\alpha_n^{(1)}$	$\alpha_n^{(2)}$	ϵ_n
10	0·3495	0·1884	−0·2651	
11	0·3276	0·1092	−0·2475	
12	0·3055	0·0629	−0·1686	
13	0·2852	0·0407	−0·0813	
14	0·2672	0·0329	−0·0138	0·0356
15	0·2515	0·0320	−0·0262	0·0219
16	0·2378	0·0334	0·0426	−0·0222
17	0·2259	0·0346	0·0437	−0·0263
18	0·2153	0·0349	0·0372	−0·0088
19	0·2057	0·0342	0·0287	−0·0102
20	0·1971	0·0329	0·0211	−0·0095
21	0·1892	0·0312	0·0155	−0·0102
22	0·1819	0·0295	0·0118	−0·0073
23	0·1752	0·0277	0·0096	0·0164

extrapolants suggest $\gamma_{11} < 0{\cdot}01$. Analysis of the untransformed series suggests a value close to 0·00 and we take as our final estimate

$$\gamma_{11} = 0{\cdot}00 \pm 0{\cdot}01. \tag{3.3}$$

The exact result is $\gamma_{11} = 0{\cdot}00$ (McCoy and Wu 1973), and these results, together with the bulk exponent values $\gamma = \frac{7}{4}$ and $\nu = 1$, satisfy both surface and RG scaling.

Following Barber *et al* (1978) we have made a direct test of surface and RG scaling by forming a series whose divergence is characterised by a 'breakdown of scaling exponent' $\phi = 2\gamma_1 - \gamma_{11} - \gamma - \nu$. For surface scaling to hold, we require $\phi \equiv 0$. Similarly, the exponent $\theta = \gamma_{11} - \nu + 1$ should be zero if RG scaling is to hold. Such a series can be formed from the coefficients of known series. Writing the bulk susceptibility series χ and the second spherical moment series μ_2 as

$$\chi = \sum_{n\geq 0} c_n v^n \qquad \mu_2 = \sum_{n\geq 0} d_n v^n$$

and observing that $c_n \sim \mu^n n^{\gamma-1}$, $d_n \sim \mu^n n^{\gamma+2\nu-1}$, $c_n^{(1)} \sim \mu^n n^{\gamma_1-1}$ and $c_n^{(1,1)} \sim \mu^n n^{\gamma_{11}-1}$, it is clear that

$$e_n = [c_n^{(1)}]^2/[c_n^{(1,1)}(c_n d_n)^{1/2}] \sim n^{\phi} \tag{3.4}$$

and that

$$f_n = n^{\gamma+1} c_n^{(1,1)}/[c_n d_n]^{1/2} \sim n^{\theta}. \tag{3.5}$$

From the sequences $\{e_n\}$ and $\{f_n\}$ we can estimate ϕ and θ both from the sequences $\{\phi_n\}$, where

$$\phi_n = \frac{n}{2}[e_n/e_{n-2} - 1] \tag{3.6}$$

and the sequence of linear extrapolants $\{\phi_n^{(1)}\}$, where

$$\phi_n^{(1)} = \tfrac{1}{2}[n\phi_n - (n-2)\phi_{n-2}]. \tag{3.7}$$

Sequences $\{\theta_n\}$ and $\{\theta_n^{(1)}\}$ are defined by (3.6) and (3.7) if e_n is replaced by f_n. In forming these sequences we have used the bulk susceptibility series given by Sykes *et al* (1972) and the second moment series derived by B G Nickel (1979, private communication).

The sequences defined above are shown in table 4, from which we can estimate $\phi = 0{\cdot}00 \pm 0{\cdot}02$ and $\theta = 0{\cdot}00 \pm 0{\cdot}01$, in agreement with the expected results $\theta = \phi = 0{\cdot}0$.

Table 4. Direct tests of the scaling relations. For scaling to hold, $\phi_n^{(1)}$ and $\theta_n^{(1)}$ should approach zero.

n	ϕ_n	$\phi_n^{(1)}$	θ_n	$\theta_n^{(1)}$
10	−0·080 99	0·045 11	0·5656	−0·092 43
11	−0·040 34	0·061 40	0·4743	−0·079 20
12	−0·063 12	0·026 22	0·4649	−0·038 49
13	−0·036 95	−0·018 33	0·4046	0·021 45
14	−0·052 36	0·012 17	0·3961	−0·016 99
15	−0·031 77	0·001 92	0·3517	0·007 56
16	−0·043 00	0·022 55	0·3457	−0·006 95
17	−0·028 28	−0·002 12	0·3118	0·012 88

4. Discussion

The significance of the above analysis is not the analysis of the χ_{11} series, since the exponent is already known exactly. Rather, by repeating the method of analysis used in the analogous SAW problem for which the exponents are not known exactly, we are able to assess the reliability of the method of analysis. Since we obtained good agreement with the known results in the Ising case, we are more confident of the earlier result of Barber *et al* (1978) that RG scaling fails for the square lattice SAW model. Recently

Whittington *et al* (1980) showed that the surface susceptibility exponent γ_s was slightly different from the scaling value $\gamma_s = \gamma + \nu$, so these two examples of the breakdown of scaling for the square lattice SAW model indicate that there may be something rather special about the $n = 0$ limit of the n-vector Hamiltonian when translational invariance is destroyed.

Extending and analysing the γ_1 series enabled us to make the estimate $\gamma_1 = 1{\cdot}375 \pm 0{\cdot}005$, compared with the earlier estimate (Whittington *et al* 1979a) of $\gamma_1 = 1{\cdot}372 \pm 0{\cdot}01$. This is in precise agreement with the estimate of $\gamma_1 = 1\frac{3}{8}$ from surface scaling, and with the estimate obtainable from the scaling relation $\gamma = \nu(2 - \eta_\perp)$ given by Binder and Hohenberg (1972) when coupled with the recent exact result $\eta_\perp = \frac{5}{8}$ obtained by Kroemer and Pesch (1979).

Finally, we remark that the series derivation is a nice example of the applicability of the appropriately generalised finite lattice method.

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