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Ising model amplitudes and extended lattice–lattice scaling

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Abstract. Extended lattice–lattice scaling (that is, universality of scaling corrections) is investigated for the two- and three-dimensional Ising models. It is shown to break down for non-Archimedean lattices in two dimensions, and for all lattices in three dimensions. In the course of the investigation several new higher order amplitudes for the two- and three-dimensional Ising models are obtained. These include an exact evaluation of the amplitude of the second most singular term of the susceptibility of the Kagomé lattice, for which we find $C_1^+ = 0{\cdot}086936625$, $C_1^- = -0{\cdot}0023063996$.

1. Introduction

This paper continues and refines the investigation commenced in two earlier papers (Guttmann 1975a, b, to be referred to as I and II respectively), devoted to a study of the nearest-neighbour spin-$\frac{1}{2}$ Ising model susceptibility amplitudes in two and three dimensions.

Lattice–lattice scaling, which relates the amplitudes of the most singular part of the free energy and its field and temperature derivatives on one lattice to the corresponding quantity on another lattice, was first introduced by Betts *et al* (1971). Its validity in an extended form, when applied to the amplitudes of the second most singular term was tacitly assumed by Guttmann (1974) for a number of two-dimensional Ising lattices. Ritchie and Betts (1975) studied explicitly formulated extended lattice–lattice scaling and showed that while it held for the square, triangular and honeycomb lattices, it did not hold for the Kagomé lattice.

For the Kagomé lattice we can write the zero-field isothermal susceptibility as

$$\frac{kT\chi_0(T)}{m^2} \sim \begin{cases} C_0^+(1-T_c/T)^{-7/4} + C_1^+(1-T_c/T)^{-3/4} & \\ \qquad + D_0^+ + \text{higher order terms} & T > T_c \\ C_0^-(T_c/T-1)^{-7/4} + C_1^-(T_c/T-1)^{-3/4} & \\ \qquad + D_0^- + \text{higher order terms} & T < T_c. \end{cases} \tag{1.1}$$

We calculate C_1^+ and C_1^- exactly, incidentally confirming the breakdown of lattice–lattice scaling for this lattice, and also evaluate D_0^+ and D_0^- approximately.

In a related manner we have estimated D_0^+ for the honeycomb lattice, which, in conjunction with our estimate of D_0^- in I, supports a conjecture of Barouch *et al* (1973) that $D_0^+ = D_0^-$. This conjecture is also discussed in the following section.

In § 3 a further amplitude for the susceptibility of the triangular lattice is obtained.

In § 4 we extend the work of II on three-dimensional lattices. Our results show that extended lattice–lattice scaling breaks down for all three-dimensional lattices.

2. The Kagomé lattice

As shown by Ritchie and Betts (1975) extended lattice–lattice scaling breaks down for the Kagomé lattice. It is therefore not possible to obtain the second most singular susceptibility amplitude for this lattice from the extended lattice–lattice scaling argument and the known amplitudes for the square, triangular and honeycomb lattices. However this amplitude can be estimated from the following expression which relates the reduced susceptibility of the Kagomé lattice to that of the honeycomb lattice:

$$\chi_{\mathrm{K}}(Q)=\frac{3}{2}\left(1-\frac{4}{(\mathrm{e}^{4Q}+1)^2}\right)\chi_{\mathrm{h}}(K)+\frac{1}{2}\left[\left(1+\frac{4}{(\mathrm{e}^{4Q}+1)^2}\right)-\left(1-\frac{4}{(\mathrm{e}^{4Q}+1)^2}\right)\epsilon_{\mathrm{h}}(K)\right]. \tag{2.1}$$

The subscripts K and h refer to the Kagomé and honeycomb lattices, $Q=J/kT_{\mathrm{K}}$ and $K=J/kT_{\mathrm{h}}$ are the dimensionless temperature variables for the two lattices and $\epsilon_{\mathrm{h}}(K)$ is the nearest-neighbour spin correlation function for the honeycomb lattice. This expression was first given in a slightly less accessible form by Sykes and Zucker (1961) and was more recently given, with several minor errors, by Syozi (1972).

From this expression, we obtain for the Kagomé lattice,

$$C_0^+=1\cdot0181422309 \qquad C_1^+=0\cdot086936625$$

$$C_0^-=0\cdot0270109734 \qquad C_1^-=-0\cdot0023063996.$$

Extended lattice–lattice scaling gives the same values for $C_0^{\pm}$ but gives values for $C_1^{\pm}$ which are arithmetically 1·3984% larger. It is noteworthy that $C_1^+/C_1^-=-37\cdot693652=-C_0^+/C_0^-$ for the Kagomé lattice, as well as for the square, triangular and honeycomb lattices (Guttmann 1974).

From (2.1) we can also obtain an expression for D_0^+ for the Kagomé lattice ($D_{0\mathrm{K}}^+$) in terms of the corresponding quantity ($D_{0\mathrm{h}}^+$) for the honeycomb lattice. Thus we find

$$D_{0\mathrm{K}}^+=(4\surd3-6)(1\cdot5D_{0\mathrm{h}}^++1/3\surd3), \tag{2.2}$$

since $\epsilon_{\mathrm{h}}(K_{\mathrm{c}})=4\surd3/9$ (Syozi 1972).

In I we estimated $D_{0\mathrm{h}}^+\approx-0\cdot24$. As we now show, it is possible to improve this estimate. The following expression connecting the susceptibilities on the triangular and honeycomb lattices:

$$\chi_{\mathrm{t}}(w)=\tfrac{1}{2}(\chi_{\mathrm{h}}(v)+\chi_{\mathrm{h}}(-v)) \tag{2.3}$$

was first given by Fisher (1959), where $w=\tanh(J/kT_{\mathrm{t}})$ is the triangular lattice temperature variable and $v=\tanh(J/kT_{\mathrm{h}})=[w(1+w)/(1+w^3)]^{1/2}$. From (2.3) we immediately obtain

$$D_{0\mathrm{t}}^+=\tfrac{1}{2}(D_{0\mathrm{h}}^++\chi_{\mathrm{h}}(-v)) \tag{2.4}$$

where $\chi_{\mathrm{h}}(-v_{\mathrm{c}})=0\cdot1224\pm0\cdot0003$ (Sykes *et al* 1972) and $D_{0\mathrm{t}}^+=-0\cdot0496\pm0\cdot002$ (see I), so that $D_{0\mathrm{h}}^+=-0\cdot222\pm0\cdot004$. From this result and (2.2) we obtain $D_{0\mathrm{K}}^+=-0\cdot131\pm0\cdot006$.

In I we investigated a conjecture of Barouch *et al* (1973) that $D_0^+=D_0^-$ for the two-dimensional Ising model on a square lattice, and found it well confirmed numerically both for the square and triangular lattices. We also obtained $D_{0\mathrm{h}}^-=0\cdot24^{+0\cdot02}_{-0\cdot03}$

which, when combined with our present estimate $D_{0h}^{+}=-0\cdot 222\pm 0\cdot 004$ also supports $D_0^+=D_0^-$ for the honeycomb lattice. Actually the truth of this conjecture is hardly surprising, since we can write the susceptibility as follows:

$$\chi(T)=\chi_s(T)+\chi_r(T) \tag{2.5}$$

where $\chi_s(T)$ is the singular part of the susceptibility and diverges as $T\to T_c$, while $\chi_r(T)$ is the regular part of the susceptibility and $\lim_{T\to T_c}\chi_r(T)$ exists. The conjecture $D_0^+=D_0^-$ is then simply a statement that $\chi_r(T)$ is continuous at $T=T_c$. That is, in addition to the existence of $\lim_{T\to T_c}\chi_r(T)$, we require that the limit is equal to $\chi_r(T_c)$. $\chi(T)$ would have to be functionally pathological for this to be false, so it is entirely reasonable to assume the truth of the conjecture $D_0^+=D_0^-$, so we thereby obtain $D_{0K}^-=-0\cdot 131\pm 0\cdot 006$.

Notice however that (2.5) and associated statements are by no means trivial. For example it may be tempting to write $\chi_s(T)\sim(1-T_c/T)^{-7/4}\phi(T)$ where ϕ is assumed regular at $T=T_c$. Such a simple functional form cannot be the case for both the honeycomb and the triangular lattices, as is clear from the calculation in the next section.

3. The triangular lattice

In I we wrote the triangular lattice high-temperature susceptibility as

$$\frac{kT\chi_0(T)}{m^2}\sim C_{0t}^{+}(1-T_c/T)^{-7/4}+C_{1t}^{+}(1-T_c/T)^{-3/4}+C_{2t}^{+}(1-T_c/T)^{1/4}$$
$$+\mathrm{O}[(1-T_c/T)^{5/4}]+D_{0t}^{+}+D_{1t}^{+}(1-T_c/T)+\mathrm{O}[(1-T_c/T)^2]. \tag{3.1}$$

From (2.3) however, it is clear that additional terms may be present, since as $w\to w_c$, $v\to v_c$ and

$$\chi_h(-J/kT)\sim F_{0,h}(1-T_c/T)\ln(1-T_c/T)+F_{1,h}+\cdots, \tag{3.2}$$

while

$$\chi_h(J/kT)\sim C_{0,h}^{+}(1-T_c/T)^{-7/4}+C_{1,h}^{+}(1-T_c/T)^{-3/4}+D_{0,h}^{+}+\cdots. \tag{3.3}$$

This would imply the addition of a term of the form

$$F_{0,t}(1-T_c/T)\ln(1-T_c/T) \tag{3.4}$$

to (3.1). Since $F_{0,h}=0\cdot 182\pm 0\cdot 001$ (Sykes *et al* 1972), it follows after some algebra that $F_{0,t}=0\cdot 0527\pm 0\cdot 003$. Alternatively, (3.3) may contain a term $-F_{0,h}(1-T_c/T)\ln(1-T_c/T)$ which would imply that $F_{0,t}$ in (3.4) is precisely zero. It follows then that $\chi_s(T)=(1-T_c/T)^{-7/4}\phi(T)$ where $\phi(T)$ is regular at $T=T_c$ cannot be true for *both* the triangular and the honeycomb lattices.

4. Three-dimensional lattices

It is known that extended lattice–lattice scaling breaks down for the two-dimensional Kagomé lattice and for the three-dimensional tetrahedral lattice (Oitmaa and Ho-Ting-Hun 1976). Both these lattices are non-Archimedean. That is, the tesselations incident upon each lattice site are not all identical. This is in contrast to the square, triangular and honeycomb lattices in two dimensions and to the three standard cubic lattices in three dimensions. An equivalent statement is that the coordination number of the dual lattice is not constant.

Since extended lattice–lattice scaling *does* hold for Archimedean two-dimensional lattices, this observation suggests that it is worthwhile to investigate extended lattice–lattice scaling for Archimedean three-dimensional lattices. An attempt in this direction was made in II, where the high-temperature susceptibility series were investigated. Unfortunately, given the available series coefficients, it was only possible to estimate C_1^+ for the face-centred cubic (FCC) lattice. It is however possible to estimate the next most singular term for the spontaneous magnetisation for all the standard three-dimensional lattices. We tentatively write the spontaneous magnetisation as

$$I_0(T) \approx B_0(T_c/T-1)^{\beta} + B_1(T_c/T-1)^{1+\beta} + \dots \tag{4.1}$$

where $\beta = \frac{5}{16}$, with B_0 and T_c lattice dependent and given in II. Next, we form the series

$$f(u) = I_0(u) - D_0(1-u/u_c)^{\beta} \sim D_1(1-u/u_c)^{1+\beta}, \tag{4.2}$$

where $u = \exp(-4J/kT)$ is the usual low-temperature expansion variable, and D_0 is simply related to B_0. We found that Padé approximants to the logarithmic derivative of $f(u)$ had well defined poles at $u = u_c$, with residues within a few per cent of $1\frac{5}{16}$. This confirms the functional form assumed in (4.1) and (4.2). That is, the correction to scaling exponent of the spontaneous magnetisation is one, as tentatively assumed in writing (4.1). To conserve space these approximants are not shown. In order to estimate D_1, and hence B_1, we next formed Padé approximants to

$$(u_c - u)[-f(u)]^{-1/1+\beta}|_{u=u_c}.$$

The approximants so obtained are shown for the simple cubic lattice in table 1. From

Table 1. Padé approximants to $(u_c - u)[-f(u)]^{-16/21}$ for the simple cubic lattice where $f(u)$ is given by (4.2).

N	$[N/N-1]$	$[N/N]$	$[N/N+1]$
4	0·34713	0·34440	0·34249
5	0·33414	0·34378	0·34720
6	0·34481	0·34489	0·34507
7	0·34475	0·34513	0·34510
8	0·34509	0·34511	0·34510
9	0·34511	0·34513	0·34507
10	0·34506	0·34524	

this table we estimate the limit to be $0{\cdot}3450 \pm 0{\cdot}0005$, from which follows $B_1 = -1{\cdot}296 \pm 0{\cdot}003$. Similarly well converged Padé tables were obtained for the same quantity for the diamond, BCC and FCC lattices. The results are summarised below:

$$B_1 = -1{\cdot}770 \pm 0{\cdot}014 \text{ (diamond)} \qquad B_1 = -1{\cdot}296 \pm 0{\cdot}003 \text{ (SC)}$$

$$B_1 = -1{\cdot}040 \pm 0{\cdot}004 \text{ (BCC)} \qquad B_1 = -0{\cdot}9784 \pm 0{\cdot}0013 \text{ (FCC)}.$$

The quoted errors include both confidence limits on the extrapolated Padé tables and the uncertainty in the values of u_c and B_0 quoted in II. As discussed in II, the ratio (B_0/B_1) for lattice X divided by (B_0/B_1) for the FCC lattice should equal g_{FCC}/g_X, where g_X is the temperature scaling parameter for lattice X. Values of g_X are given in II. The values of this quotient and of g_{FCC}/g_X are shown in table 2. It can be seen that the figures disagree by 10% for the diamond lattice, by 5% for the SC lattice and by 0·6% for the BCC lattice.

Table 2. Numerical estimates of observed spontaneous magnetisation amplitude ratios compared to ratios predicted by extended lattice–lattice scaling.

Lattice	B_0/B_1	$(B_0/B_1)/(B_0/B_1)_{FCC}$	g	g_{FCC}/g
Diamond	$-0{\cdot}943\pm0{\cdot}008$	$0{\cdot}621\pm0{\cdot}006$	$1{\cdot}448\pm0{\cdot}008$	$0{\cdot}691\pm0{\cdot}004$
SC	$-1{\cdot}211\pm0{\cdot}003$	$0{\cdot}797\pm0{\cdot}004$	$1{\cdot}191\pm0{\cdot}004$	$0{\cdot}840\pm0{\cdot}003$
BCC	$-1{\cdot}448\pm0{\cdot}006$	$0{\cdot}953\pm0{\cdot}006$	$1{\cdot}043\pm0{\cdot}005$	$0{\cdot}959\pm0{\cdot}005$
FCC	$-1{\cdot}519\pm0{\cdot}003$	1	1	1

Clearly then, the extended lattice–lattice scaling does not hold even for the Archimedean lattices in three dimensions, unlike the situation in two dimensions. Note however that the breakdown is only a few per cent, as anticipated in II. Thus extended lattice–lattice scaling is still likely to form a useful predictive tool for Archimedean lattices in three dimensions, with the *proviso* that estimates so obtained are likely to be in error by a few per cent. In many instances, for example the second most singular term of the high-temperature susceptibility series C_1^+, this is still considerably more accurate than any estimates obtainable by direct series analysis.

In order to investigate extended lattice–lattice scaling further, it would be highly desirable to have extended high-temperature susceptibility series available, so that better direct estimates of C_1^+ could be made.

For the non-Archimedean tetrahedral lattice studied by Oitmaa and Ho-Ting-Hun (1976) the breakdown in extended lattice–lattice scaling is much more substantial.

5. Conclusions

A number of new amplitudes have been obtained for the two- and three-dimensional

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