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LETTER TO THE EDITOR

The mean size of Ising clusters: a confluent singularity analysis

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Abstract. We re-examine, using a confluent singularity analysis, existing low-temperature series for the mean size of finite clusters for the pure spin-$\frac{1}{2}$ nearest-neighbour Ising model in two dimensions. Although the triangular lattice is problematical, results for the honeycomb and square lattices may be interpreted as indicating a dominant exponent $\theta = 1.87 \pm 0.04$ (consistent with the theoretical prediction $\theta = \gamma + \beta$), together with competing analytic and non-analytic ($\Delta_1 = 1.35 \pm 0.25$) correction-to-scaling terms.

In this letter we re-analyse existing low-temperature series expansions (Sykes and Gaunt 1976) for the mean size of finite clusters for the pure spin-$\frac{1}{2}$ nearest-neighbour Ising model in $d = 2$ dimensions. However, in contrast to the earlier work, we include in our analysis the possibility of confluent correction-to-scaling terms.

The motivation for this work was provided by recent speculation regarding the critical exponent θ which characterises the dominant singular behaviour of the mean cluster size S. The speculation stems from an explicit theory of Ising systems in $d = 1 + \varepsilon$ dimensions developed, by Bruce and Wallace (1983), from the droplet phenomenology of phase transitions (Fisher 1967). As shown by Bruce and Wallace (BW), standard droplet phenomenology predicts

$$\theta = \gamma, \tag{1}$$

whilst their explicit theory leads to

$$\theta = \gamma + \beta. \tag{2}$$

Here γ and β are the usual critical exponents characterising the zero-field susceptibility and order parameter, respectively.

The prediction (2) coincides with a conjecture due to Stauffer (1977). This conjecture is based upon a scaling droplet model due to Binder (1976), the validity of which depends on the coincidence of cluster and droplet properties. BW argue that their droplet picture of the Ising phase transition should be valid for ε sufficiently small, i.e. in sufficiently low space dimensions. It seems likely that dimension $d = 3$ is not low enough since Monte Carlo (Müller-Krumbhaar 1974) and series studies (Sykes and Gaunt 1976) have established that Ising clusters percolate at a temperature below the Curie temperature T_c. It is difficult therefore to identify clusters with droplets (whose size should diverge only at T_c). In $d = 2$ dimensions, however, it has been proved (Coniglio *et al* 1977) that the percolation of Ising clusters with nearest-neighbour interactions only occurs at the critical temperature, suggesting that the critical properties of clusters and droplets might coincide. The consequences of this identification can

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be tested by using the estimate

$$\theta = 1.91 \pm 0.01 \qquad d = 2 \tag{3}$$

obtained by Sykes and Gaunt (1976) from biased dlog Padé approximant studies for the triangular lattice. Although this result is inconsistent with the phenomenological prediction (1), $\theta = \gamma = 1.75$, it is fairly close to the prediction (2) of BW, $\theta = \gamma + \beta = 1.875$. (We have used the exact $d = 2$ values for γ and β.)

Although the discrepancy between (3) and (2) is small (less than 2%), it is 3.5 times larger than the uncertainty quoted in (3). It is clearly of crucial importance to decide if this discrepancy is real, or simply arises because the uncertainties in the numerical estimate (3) are unrealistically small. A persistent discrepancy would presumably have fatal consequences for the explicit droplet theory of BW in two dimensions—at least in its present form. On the other hand and not unnaturally, therefore, BW are inclined to mistrust the estimate in (3). They speculate that the series expansions may be too short to take proper account of the 'droplets within droplets' structure which is an essential ingredient of their (and any scale invariant) picture of the critical region.

To be specific, Sykes and Gaunt (1976) assumed that

$$S(u) \sim C(u_c - u)^{-\theta} \qquad (u \to u_c -) \tag{4}$$

where $u = \exp(-4J/kT)$ is a low-temperature Ising variable, u_c is its (exactly known) value at T_c and C is a constant amplitude. Series expansions were derived† through u^{17}, z^{14} $(z^2 = u)$ and u^{10} for the triangular, honeycomb and square lattices, respectively. The series were analysed using the ratio and biased dlog Padé approximant techniques (Gaunt and Guttmann 1974). Here we replace (4) by an asymptotic form which includes both analytic and non-analytic correction-to-scaling terms:

$$S(u) \sim C(u_c - u)^{-\theta}[1 + A(u_c - u)^{\Delta_1} + B(u_c - u)], \tag{5}$$

where A and B are non-universal amplitudes and Δ_1 is the dominant non-analytic correction-to-scaling exponent.

Presumably $S(u)$ is in the $d = 2$ Ising universality class. Within the renormalisation group (RG) framework, *analytic* correction terms, such as $B(u_c - u)$, arise (Aharony and Fisher 1980, 1983) from the nonlinearity of the scaling fields and not from the leading irrelevant variables. Estimates of the *non-analytic* correction-to-scaling exponent Δ_1, calculated by RG methods, include

$$\Delta_1 = \begin{cases} 1.4 \pm 0.8 & \text{(Baker } et\ al \text{ 1978‡)} \\ 1.3 \pm 0.2,\ 1.40 & \text{(Le Guillou and Zinn-Justin 1980).} \end{cases} \tag{6}$$

Although predicted by RG theory, non-analytic terms have never been observed for the spin-$\frac{1}{2}$ $d = 2$ nearest-neighbour Ising model. For all the functions studied so far, their amplitude vanishes. However, their presence in $d = 2$ systems in the Ising universality class has been reported. Thus, for the spin-1 Ising and hard-square models, Adler and Enting (1984) have used 45 and 24 term series, respectively, to estimate

$$1.0 < \Delta_1 < 1.3. \tag{7}$$

† Note that our S corresponds to S^* in the notation of Sykes and Gaunt.

‡ This 'corrected' value is quoted by Adler and Enting (1984), Barma and Fisher (1984) and Baker and Johnson (1984).

Barma and Fisher (1984, 1985) have used partial differential approximants to study 21 term (two-variable) series for the Klauder and double Gaussian models both of which are believed to be in the Ising universality class. They conclude that

$$\Delta_1 = 1.35 \pm 0.25. \tag{8}$$

Using not entirely rigorous arguments, Nienhuis (1982) has conjectured $\Delta_1 = \frac{4}{3}$ but, as argued by Barma and Fisher, the interpretation of this result may be subtle.

In this letter, we re-analyse the existing series for $S(u)$ using a method employed extensively by Adler and by Privman (see, e.g., Adler *et al* 1983, Privman 1983, Adler and Enting 1984). Barma and Fisher (1985) have criticised any *single*-variable analysis in which the critical point is not known exactly because of the difficulty in disentangling reliably the effects of irrelevant operators from those due to the nonlinear scaling fields. Fortunately, in our case, the exact critical point *is* available and we find some *tentative* evidence for the presence of non-analytic (as well as analytic) correction-to-scaling terms confluent with a dominant exponent θ whose value is consistent with the prediction $\theta = \gamma + \beta = 1.875$.

In this method the original series in u is first transformed to one in

$$y = 1 - (1 - u/u_c)^{\Delta},$$

after which the series for

$$G_{\Delta}(y) = \Delta(1-y)(\mathrm{d}/\mathrm{d}y) \ln S(y)$$

is calculated for a range of values of Δ. For each value of Δ, estimates of θ are obtained by evaluating several central Padé approximants to $G_{\Delta}(y)$ at $y = 1$. One might anticipate, and experience with test series confirms (Privman 1983), a region of convergence in the (θ, Δ) plane around the correct (θ, Δ_1) point. Plots obtained by this technique are given in figures 1, 2 and 3 for the honeycomb, square and triangular lattices, respectively. In interpreting these figures, we have been guided by comparison with the known behaviour of test series.

For the honeycomb lattice (figure 1), there is a rather broad region of convergence centred around $\Delta \sim 1.35$, $\theta \sim 1.87$ and a 'weak' pole structure (Privman 1983) at $\Delta \leqslant 1$.

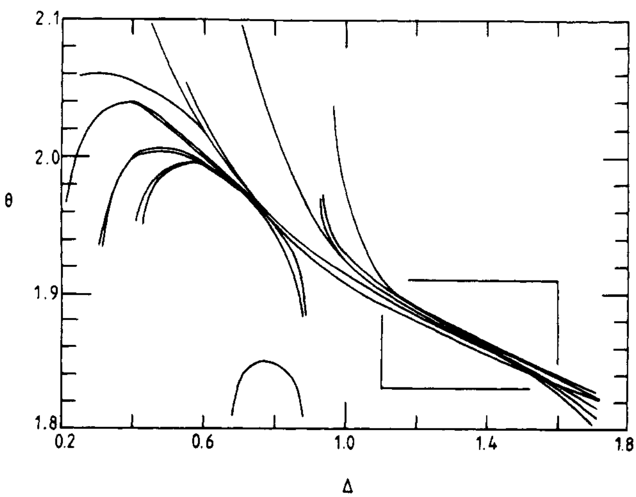

Figure 1. $\theta(\Delta)$ plot for the mean size of Ising clusters on the honeycomb lattice.

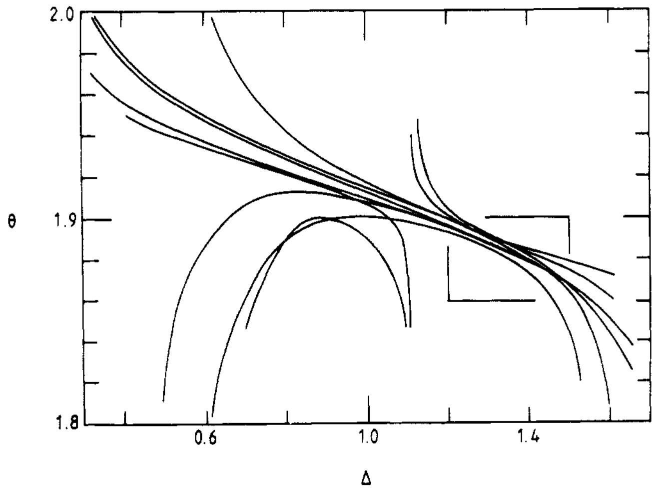

Figure 2. $\theta(\Delta)$ plot for the mean size of Ising clusters on the square lattice.

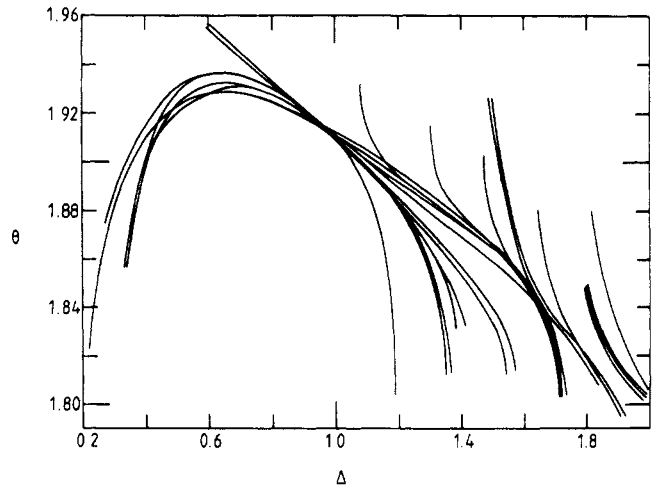

Figure 3. $\theta(\Delta)$ plot for the mean size of Ising clusters on the triangular lattice.

In the case of the square lattice (figure 2), there is a convergence region close to $\Delta \sim 1.35$, $\theta \sim 1.88$ with a weak pole structure at $\Delta \geqslant 1$. The behaviour of the honeycomb and square lattices is thus rather similar, namely a convergence region around $\Delta \sim 1.35$, $\theta \sim 1.87$–1.88 with a weak pole structure not far from $\Delta = 1$.

The behaviour observed for the triangular lattice (figure 3) is rather different. There is now a 'broad' pole structure at $\Delta \sim 1.4$ and a convergence region lying close to $\Delta = 1$ with a corresponding exponent of 1.91. Since $\Delta = 1$ is equivalent to the usual biased dlog Padé analysis, this explains why the estimate (3) of Sykes and Gaunt was so precise. However, the presence of the very broad pole structure near $\Delta \sim 1.4$ suggests to us that the convergence region at $\Delta = 1$ may not correspond to an accurate estimate of the dominant exponent θ and that, consequently, Sykes and Gaunt may have underestimated the uncertainties in (3). We have found such an interpretation to be consistent with our own extensive study of test series. Similar behaviour is also exhibited in figure 3 of Privman (1983).

In summary, we have employed a method much used by Adler and by Privman to reanalyse existing low-temperature series expansions for the mean size of Ising clusters in $d = 2$ dimensions. This is the first attempt to take account of confluent correction-to-scaling terms for these series. Although the results are difficult to interpret and not particularly impressive, they are more revealing than those obtained with the biased dlog Padé and ratio techniques alone. For example, from figure 3, which is for the triangular lattice, we can understand from the convergence region at $\Delta = 1$ how the high precision estimate (3) for the dominant exponent θ first arose. However, as mentioned above, the study of test series reveals that the presence of a broad pole structure (such as that exhibited in figure 3 near $\Delta_1 \sim 1.4$) can seriously affect the reliability of such plots in neighbouring convergence regions and thus lead to over-optimistic uncertainty estimates. On the other hand, there are no such broad pole structures for the honeycomb and square lattices, so from the convergence regions indicated in figures 1 and 2 we estimate

$$\theta = 1.87 \pm 0.04, \tag{9}$$

with a non-analytic correction-to-scaling term having an exponent

$$\Delta_1 = 1.35 \pm 0.25. \tag{10}$$

The estimate (9), unlike the previous estimate (3), is consistent with the prediction $\theta = \gamma + \beta = 1.875$. The estimate (10) is identical with the series estimate, (8), for the Klauder and double Gaussian models and is consistent with the RG estimates, (6), the series estimate, (7), for the spin-1 Ising and hard-square models, and with the Nienhuis conjecture $\Delta_1 = \frac{4}{3}$. Assuming our interpretation of figures 1 and 2 is correct, this seems to be the first time that non-analytic correction-to-scaling terms have been detected for the *pure* $d = 2$ spin-$\frac{1}{2}$ nearest-neighbour Ising model. We speculate that a possible explanation may somehow be related to the fact that while other work has concentrated on thermodynamic functions (such as the zero-field susceptibility), the mean size studied here characterises a 'geometrical' property of Ising clusters.

As we have seen, the plots are very difficult to interpret, particularly as the series are of different lengths and there is competition between the leading analytic and non-analytic correction terms with their relative strengths changing from lattice to lattice. (For example, the convergence region near $\Delta = 1$ in figure 3 *may* indicate that the analytic correction term has a relatively larger amplitude for the triangular lattice than it has for the honeycomb and square lattices.) The effect of higher-order corrections is also hard to assess. However, at the very least, we believe our work shows that the theoretical prediction $\theta = \gamma + \beta$ and the existing series expansion data are not necessarily inconsistent. A discrepancy of around 2% may be accounted for by the neglect of confluent correction-to-scaling terms.

It has been suggested that additional uncertainties due to the shortness of the series and the consequent inadequate treatment of the nested droplet structure are also possible. In this context, BW point out that a study which (accidentally or deliberately) includes, in the definition of cluster size, *all* the lattice sites contained within a cluster boundary (sites which may accommodate nested clusters) will yield a cluster size exponent $\theta' > \theta$. However, Sykes and Gaunt (1976) did *not* use such a definition. In their definition of cluster size, the size of a connected configuration of 'down' spins depends only on the number of 'down' spins in that configuration. Furthermore, we note that it is very easy for a connected cluster of 'down' spins to contain within its boundary a connected cluster of 'up' spins but be, nevertheless, too small to accommodate a nested cluster of 'down' spins. (On the triangular lattice, the simplest example is a hexagon of six 'down' spins surrounding a connected cluster of one 'up' spin.) A connected cluster of 'down' spins must be quite large before it can accommodate even the smallest nested cluster, namely a single 'down' spin. On the triangular lattice, a single 'down' spin can just be nested inside a connected cluster of twelve 'down' spins in the shape of a regular hexagon. However, this configuration does not contribute to the $S(u)$ series until u^{27}, which is well beyond the last available coefficient, u^{17}. Similarly, for the honeycomb and square lattices, the simplest nested clusters do not contribute until z^{21} and u^{18}, respectively, whereas the last available terms are z^{14} and u^{10}. In other words, nested clusters have not so far contributed to any of the series studied here. Nevertheless, the existing series are capable of yielding what is presumably the correct result ($\theta = \gamma + \beta$). Evidently, the key thing is for the series expansions to capture a good estimate for the distribution of holes within a droplet so that the true droplet volume (i.e. the number of 'down' spins it contains) must be correctly estimated.

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References

Adler J and Enting I G 1984 *J. Phys. A: Math. Gen.* **17** 2233
Adler J, Moshe M and Privman V 1983 *Percolation Structures and Processes* ed G Deutscher, R Zallen and J Adler (Bristol: Adam Hilger) p 397
Aharony A and Fisher M E 1980 *Phys. Rev. Lett.* **45** 679
—— 1983 *Phys. Rev.* B **27** 4394
Baker G A Jr and Johnson J D 1984 *J. Phys. A: Math. Gen.* **17** L275
Baker G A Jr, Nickel B G and Meiron D I 1978 *Phys. Rev.* B **17** 1365
Barma M and Fisher M E 1984 *Phys. Rev. Lett.* **53** 1935
—— 1985 *Phys. Rev.* B **31** 5954
Binder K 1976 *Ann. Phys., NY* **98** 390
Bruce A D and Wallace D J 1983 *J. Phys. A: Math. Gen.* **16** 1721
Coniglio A, Nappi C R, Perrugi F and Russo L 1977 *J. Phys. A: Math. Gen.* **10** 205
Fisher M E 1967 *Physics* **3** 255
Gaunt D S and Guttmann A J 1974 *Phase Transitions and Critical Phenomena* vol 3, ed C Domb and M S Green (New York: Academic) p 181
Le Guillou J C and Zinn-Justin J 1980 *Phys. Rev.* B **21** 3976
Müller-Krumbhaar H 1974 *Phys. Lett.* **50A** 27
Nienhuis B 1982 *J. Phys. A: Math. Gen.* **15** 199
Privman V 1983 *J. Phys. A: Math. Gen.* **16** 3097
Stauffer D 1977 *J. Phys. A: Math. Gen.* **10** L71
Sykes M F and Gaunt D S 1976 *J. Phys. A: Math. Gen.* **9** 2131