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A note on the mean size of clusters in the Ising model

M F Sykes and D S Gaunt
Wheatstone Physics Laboratory, King's College, Strand, London WC2R 2LS, UK

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Abstract. The derivation of series expansions for the mean size of finite clusters in the Ising model is described briefly. From an analysis of low temperature series it is concluded that for a two-dimensional lattice in zero magnetic field the mean size probably diverges at the Ising critical temperature, T_c, as $(T_c - T)^{-\theta}$, with $\theta = 1{\cdot}91 \pm 0{\cdot}01$. It appears therefore that $\theta > \gamma' = 1{\cdot}75$ the corresponding Ising susceptibility exponent. For a three-dimensional lattice it is tentatively concluded that the mean size diverges at some temperature $T^* < T_c$.

1. Introduction

In a recent paper Coniglio (1975) has calculated the percolation probability and mean cluster size for a mixture of 'up' and 'down' spins on a simple Bethe lattice with nearest-neighbour ferromagnetic interactions of the Ising type. The corresponding solution for the percolation problem for a random mixture on a Bethe lattice was obtained by Fisher and Essam (1961); the investigation of Coniglio extends their results to a mixture of sites whose distribution is not random but is instead energetically determined. The more general problem of percolation in a three-dimensional Ising system has been studied by Müller-Krumbhaar (1974) using Monte Carlo techniques. In this paper we investigate the mean cluster size for the Ising model in two and three dimensions by series methods and draw some tentative conclusions.

The existence of a percolation threshold in many-body systems is an important phenomenon in the theory of dilute ferromagnets and inhomogeneous conductors (Kasteleyn and Fortuin 1969, Essam 1973, Kirkpatrick 1973, Essam and Fisher 1963, Griffiths and Lebowitz 1968). A study of cluster size in the Ising model is a first step towards a proper treatment of the percolation problem when interactions cannot be neglected. The interest in such a study consists not only in generalizing the percolation problem to such systems but in the investigation of the connection between phase transitions and percolation.

2. Derivation of series expansions

The elementary derivation of series expansions for *random* mixtures has been described by Sykes and Glen (1976) and Sykes *et al* (1976a, b, c), to be referred to as I–IV; the perimeter method there used is not immediately applicable to the present problem and we have had recourse to the alternative direct derivation, described in the specialized articles of Sykes and Essam (1964) and Essam and Sykes (1966), based on a knowledge of the embeddings of multicomponent graphs. We have combined this technique with the direct configurational method for series development in the Ising model described by Sykes *et al* (1965, 1973a, b, c, d, e, 1975a, b, c, to be referred to as I*–IX*) and by Domb (1974).

Following I*–IX* we define standard expansion variables

$$u = \exp(-4J/kT)$$
$$\mu = \exp(-2mH/kT). \tag{2.1}$$

At low temperatures, or in a high applied magnetic field, there exists an ordered state (for a ferromagnet). Small perturbations of this ordered state correspond to the occurrence of overturned spins, the probability of each perturbation being the appropriately normalized Boltzmann factor (I*, § 2 and II*, § 1).

For a lattice of N sites the number of overturned spins, N_1, (which we select as the primary species to be studied (Essam and Sykes 1966)) determines the *concentration* β defined by

$$N_1 = \beta N \tag{2.2}$$

and this is simply related to the magnetization I through

$$I = 1 - 2\beta. \tag{2.3}$$

The concentration is the expectation that a randomly chosen site will be occupied by an overturned spin. The series expansion for β is obtained by weighting the Boltzmann factors for the free energy by the number of overturned spins in each case. Explicitly we find on the plane triangular lattice

$$\beta(u, \mu) = \mu u^3 + \mu^2(6u^5 - 7u^6) + \mu^3(6u^6 + 27u^7 - 90u^8 + 58u^9) + \cdots + \mu^s sL_s(u) + \ldots. \tag{2.4}$$

The weighting by number of overturned spins corresponds formally to a differentiation with respect to the field variable (μ) and the expansion (2.4) is readily obtained in the above μ-grouped form as far as the corresponding high-field polynomials L_s are known for any lattice. Alternatively the expansion can be re-grouped in powers of u as far as the corresponding low temperature polynomials ψ_s are known. (For information on the availability of these polynomials see I*, III*–VI*, VIII* and IX*.)

We adopt the usual definition of mean size as the mean number of overturned spins connected to any overturned spin. To calculate the mean size, $S(u, \mu)$, of finite clusters of perturbed spins the expectation of each configuration that contributes to the free energy expansion must be further weighted by the size of each of its connected components and the resultant second moment normalized in the usual way to correspond to the mean size of clusters per perturbed spin. Following I, § 2 and III, § 1 we obtain the appropriate generalization of equation (1.11) of III in the form

$$S(u, \mu) = S^*(u, \mu)/\beta(u, \mu). \tag{2.5}$$

The second moment S^* does not correspond to a further differentiation with respect to μ since in the Ising model the connectivity of clusters of perturbed spins is not recorded by the variables μ and u. In general any term $\mu^s u^t$ corresponds to a set of distinct configurations with different numbers of connected components of size $a, b, c, \ldots$, each of which has a weight $a^2 + b^2 + c^2 \ldots$ and the most direct method of determining the total contribution to S^* is to go back to the underlying configurational data. In this way we find in our specific example for the triangular lattice:

$$S^* = \mu u^3 + \mu^2(12u^5 - 7u^6) + \mu^3(18u^6 + 81u^7 - 150u^8 + 58u^9) + \dots \quad (2.6)$$

The elimination of the field variable μ between (2.4), (2.5) and (2.6) yields an expansion for the mean size in powers of the concentration with coefficients that are functions of the temperature variable u. Explicitly, writing for convenience $\rho = 1/u$, we find for the triangular lattice

$$S = 1 + 6\rho\beta + (12\rho^3 - 18\rho^2 + 24\rho)\beta^2 + \dots \quad (2.7)$$

As the interaction tends to zero, $\rho \to 1$, and β may be identified with the probability, p, of the primary species in a random mixture. In the limit we recover the result for the non-interacting system (see I):

$$S = 1 + 6p + 18p^2 + \dots \quad (2.8)$$

In the limiting case of the zero-field Ising model (2.7) reduces, on substitution of the expansion for β, to a development in u only; it is convenient then to derive the expansion directly from the limiting forms of (2.4) and (2.6).

For the zero-field case we have made a detailed study of the configurational data and derived expansions for the triangular lattice through u^{17}, the simple quadratic lattice through u^{10}, the honeycomb lattice through z^{14} ($z^2 = u$) and for the face-centred cubic lattice through u^{32}.

Since we have based our numerical extrapolations on the function S^* we only quote the data in this form.

Triangular lattice

$$\begin{aligned} S^*(u) = {} & u^3 + 12u^5 + 11u^6 + 129u^7 + 192u^8 + 1\,360u^9 + 2\,490u^{10} \\ & + 14\,091u^{11} + 28\,895u^{12} + 143\,706u^{13} + 316\,431u^{14} \\ & + 1\,445\,761u^{15} + 3\,342\,624u^{16} + 14\,380\,794u^{17} + \dots \end{aligned} \quad (2.9)$$

Simple quadratic lattice

$$\begin{aligned} S^*(u) = {} & u^2 + 8u^3 + 65u^4 + 480u^5 + 3\,381u^6 + 23\,020u^7 \\ & + 153\,171u^8 + 1\,002\,180u^9 + 6\,473\,281u^{10} + \dots \end{aligned} \quad (2.10)$$

Honeycomb lattice

$$\begin{aligned} S^*(z) = {} & z^3 + 6z^4 + 27z^5 + 126z^6 + 552z^7 + 2\,370z^8 + 9\,998z^9 + 41\,583z^{10} \\ & + 170\,997z^{11} + 696\,558z^{12} + 2\,815\,755z^{13} + 11\,309\,301z^{14} + \dots \end{aligned} \quad (2.11)$$

Face-centred cubic lattice

$$\begin{aligned} S^*(u) = {} & u^6 + 24u^{11} - 13u^{12} + 72u^{15} + 378u^{16} - 600u^{17} + 243u^{18} + 384u^{19} \\ & + 1\,968u^{20} + 3\,216u^{21} - 14\,718u^{22} + 16\,332u^{23} + 7\,907u^{24} + 26\,640u^{25} \\ & - 13\,935u^{26} - 235\,744u^{27} + 549\,534u^{28} - 121\,320u^{29} + 174\,378u^{30} \\ & - 1\,071\,408u^{31} - 1\,994\,784u^{32} + \dots \end{aligned} \quad (2.12)$$

3. Series analysis

In this section we outline the series analysis for one two-dimensional lattice, the triangular, and for the face-centred cubic lattice in three dimensions. As the ratio and Padé approximant techniques that we have used are standard (Gaunt and Guttmann 1974), we merely summarize the main results of our analysis.

For the triangular lattice, we first calculate the Dlog Padé approximants to the series for $S(u)$ and $u^{-3}S^*(u)$. The rate of convergence in the vicinity of the physical singularity is found to be considerably more rapid in the latter case. Presumably dividing $S^*(u)$ by the singular but non-divergent function $\beta(u)$,as in (2.5), means that $S(u)$ has a more complicated analytic structure. Speaking loosely, we may say that $S^*(u)$ appears to be the more 'natural' function. Accordingly we omit our analysis of $S(u)$ and simply give in table 1 our results for $S^*(u)$. These indicate very strongly a singularity at the Ising critical point $u = u_c = \frac{1}{3}$ of the form

$$S^*(u) \simeq C(u_c - u)^{-\theta} \qquad (u \to u_c-). \tag{3.1}$$

Table 1. Dlog Padé estimates of u_c (and θ) derived from $u^{-3}S^*(u)$ for the triangular lattice.

n	$[n-1/n]$	$[n/n]$	$[n+1/n]$
2	0·28325 (−1·1956)	0·32659 (−1·8632)	0·33792 (−2·1355)
3	0·34118 (−2·2470)	0·34871 (−2·5794)	0·34111 (−2·2300)
4	0·34286 (−2·3030)‡	0·33750 (−2·0914)	0·32983 (−1·7124)
5	0·33290 (−1·8849)	0·33262 (−1·8701)	0·33454 (−1·9859)
6	0·33284 (−1·8823)‡	0·333248 (−1·9051)	0·333296 (−1·9081)
7	0·333304 (−1·9087)		

‡ Defect on negative axis.

Such a conclusion is not inconsistent with our general expectation that the introduction of interactions should reduce or at least not increase the non-interacting value p_c, that is

$$\beta_c \leqslant p_c = \tfrac{1}{2} \tag{3.2}$$

for the triangular lattice. If the equality holds then $\beta_c = \frac{1}{2}$, $I = 0$ and hence $u = u_c$ as we have found.

The corresponding exponent θ may be estimated either from a pole–residue plot of the data in table 1 or, as in table 2, by evaluating at $u = \frac{1}{3}$ the Padé approximants to the

Table 2. Padé estimates of θ from $(u_c - u)(d/du)\ln(S^*/u^3)$ using $u_c = \frac{1}{3}$.

n	$[n-1/n]$	$[n/n]$	$[n+1/n]$
2	2·1543	2·0269	2·0052
3	1·9681	2·1099†	1·9478
4	1·8374	1·9052	1·9075
5	1·9077	1·9011†	1·9101
6	1·9105	1·9106	1·9109
7	1·9089†		

† Defect on positive axis.

series for $(u_c - u)(d/du)\ln(S^*/u^3)$. Using these methods we conclude that

$$\theta = 1{\cdot}91 \pm 0{\cdot}01. \tag{3.3}$$

The Dlog Padé approximants also indicate the presence of a non-physical singularity at $u = -u_c$ where $S^*(u)$ diverges with an exponent of about $\frac{3}{4}$. This singularity causes a characteristic odd–even oscillation in the ratios of coefficients. Procedures for dealing with this kind of situation within the ratio method are described by Gaunt and Guttmann. Again we suppress all details since the results, while not inconsistent with the Padé approximant results, contribute nothing new.

Series analysis for the face-centred cubic lattice is complicated by the fact that the physical singularity lies outside the circle of convergence. Indeed according to the Dlog Padé approximants to $u^{-6}S^*(u)$, there appear to be at least three complex conjugate pairs of singularities within the physical disc. This situation is well known for low temperature Ising series (Guttmann 1969, Domb and Guttmann 1970, Domb 1974) and has for example prevented an effective analysis of the extensive low temperature susceptibility series that are available (Gaunt and Sykes 1973). Accordingly our results in three dimensions are only tentative.

In table 3 we give estimates of the physical singularity and corresponding exponent as derived from Dlog Padé approximants to $u^{-6}S^*(u)$. Again we work with $S^*(u)$, although in three dimensions it appears to have little if any advantage over $S(u)$, since presumably the analytic structure is very complicated in either case.

For the face-centred cubic lattice, the condition (3.2) becomes (Sykes *et al* 1976d)

$$\beta_c \leqslant p_c = 0{\cdot}198, \tag{3.4}$$

which implies that the physical singularity should occur at some temperature T^* below the Ising critical temperature; that is,

$$u^* = \exp(-4J/kT^*) < u_c = 0{\cdot}66473 \tag{3.5}$$

for the face-centred cubic lattice (Sykes *et al* 1972). Indeed the condition (3.4) enables one to estimate an upper bound for u^* by using the asymptotic form

$$I = 1 - 2\beta \simeq B(1-t)^{5/16} \qquad (t = T/T_c) \tag{3.6}$$

Table 3. Dlog Padé estimates of u^* (and θ) derived from $u^{-6}S^*(u)$ for the face-centred cubic lattice.

n	$[n-1/n]$	$[n/n]$	$[n+1/n]$
5	0·58333 (−1·2561)	0·61354 (−1·6832)	0·63032 (−2·0109)
6	0·65096 (−2·6665)	0·62568 (−1·9054)	0·62929 (−1·9887)‡
7	0·63545 (−2·1629)‡	0·60797 (−1·6601)†	0·65789 (−2·9316)
8	—	0·64162 (−2·2722)	0·65119 (−2·6351)‡
9	0·66243 (−3·2782)	0·66440 (−3·4254)	0·65904 (−3·0382)
10	0·66277 (−3·3019)‡	0·65632 (−2·8616)	0·65970 (−3·0794)†
11	0·66833 (−3·6917)†	0·69443 (−6·6824)†	0·64938 (−2·4941)
12	0·66299 (−3·3343)§	0·63912 (−1·9400)	0·60483 (−0·5063)
13	0·62636 (−1·2984)		

† Defect on positive axis.
‡ Defect on negative axis.
§ Defect in complex plane.

where the amplitude $B \simeq 1{\cdot}487$ (Domb 1974). We find

$$u^* \leqslant 0{\cdot}650. \tag{3.7}$$

We note that of the estimates in table 3 without defects, all four for $n \geqslant 11$ satisfy (3.7). This observation is rather suggestive since if the same analysis is performed (unpublished work) with the low temperature Ising susceptibility series none of the estimates satisfy (3.7).

Without further information it does not seem possible to draw more precise conclusions. It is likely however that the inequality holds in (3.7) since otherwise $\theta \simeq 2\frac{1}{2}$ as can be seen from a pole–residue plot of the estimates in table 3. We have seen that in two dimensions θ exceeds γ' by about 9% while at the critical dimension it is known (Coniglio 1975) that $\theta = \gamma' = 1$. Hence in three dimensions we might expect θ to exceed γ' $(= 1{\cdot}25)$ by between 0 and 9%,

$$1{\cdot}25 \leqslant \theta \leqslant 1{\cdot}36. \tag{3.8}$$

From the pole–residue plot, we then obtain

$$0{\cdot}625 \leqslant u^* \leqslant 0{\cdot}628 \tag{3.9}$$

which corresponds according to (3.6) to

$$0{\cdot}092 \leqslant \beta_c \leqslant 0{\cdot}102. \tag{3.10}$$

4. Conclusions

We have derived and analysed series expansions for the mean size of clusters in the Ising model. For the triangular lattice, the low temperature zero-field series seem to have a singularity located at the Ising critical point $u = u_c$ as suggested by Coniglio (1975) and Essam (1973). Our best estimate of the corresponding exponent $\theta = 1{\cdot}91 \pm 0{\cdot}01$ is close to $1\frac{11}{12}$ $(= 1{\cdot}91666\ldots)$ and we adopt this simple fraction as a convenient mnemonic. The confidence limits on our estimate, while not rigorous, do seem to exclude the possibility that $\theta = \gamma'$, the low temperature susceptibility exponent. Analysis of the rather shorter series (2.10) and (2.11) for the square and honeycomb lattices indicates that the above results are generally valid in two dimensions. Such a conclusion is not inconsistent with arguments like those based on (3.2) since for these lattices $p_c > \frac{1}{2}$ (see II).

In three dimensions $p_c < \frac{1}{2}$ for all the usual lattices (Sykes *et al* 1976d) so that an argument similar to that in (3.4) leads us to expect a singularity at $u^* < u_c$. We have found some evidence for this in the case of the face-centred cubic lattice, but in common with other low temperature series for the three-dimensional Ising model convergence is very slow. More precise results will have to await theoretical developments or longer series.

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