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LETTER TO THE EDITOR

Possible interpretation of the Sykes–Gaunt exponent for the mean cluster size near T_c

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Abstract. Sykes and Gaunt showed the mean cluster size in the two-dimensional Ising model to diverge as $(T_c - T)^{-\theta}$ with $\theta \simeq 1{\cdot}91$ larger than the Ising susceptibility exponent $\gamma = 1{\cdot}75$. This difference $\theta - \gamma$ is explained here at least partly by Binder's cluster model for critical points where $\theta \geqslant \gamma + \beta = 1{\cdot}875$.

Cluster or droplet models have for many years been used as a simple description of static and dynamic critical phenomena near second-order phase transitions (Fisher 1967, Domb 1976, Binder 1976, Kretschmer *et al* 1976). Such models assume as known the number n_l of clusters of size l where a 'cluster' for example is thought to be a small liquid droplet (within the gas phase) containing l molecules (Fisher 1967). Or the cluster may represent a group (of size l) of $\downarrow$ spins surrounded by $\uparrow$ spins in an Ising magnet. In simple models (Fisher 1967) the susceptibility or compressibility χ varies with the second moment of the cluster size distribution:

$$\chi \propto \sum_{l=1}^{\infty} l^2 n_l.$$

For $T \to T_c$, the susceptibility χ diverges as $|T - T_c|^{-\gamma}$ where $\gamma = 1{\cdot}75$ exactly in the two-dimensional Ising model (Wu *et al* 1976). On the other hand Sykes and Gaunt (1976) recently found near the Curie temperature of this model

$$\sum_{l=1}^{\infty} l^2 n_l \propto (T_c - T)^{-\theta}, \qquad \theta = 1{\cdot}91 \pm 0{\cdot}01 \tag{1}$$

from exact 'series expansion' analysis of n_l for small l. The aim of the present letter is to explain this difference between the exponents θ and γ for the second moment and susceptibility, respectively.

The magnetization m (in units of the saturation magnetization) follows near T_c a scaling homogeneity law: $m(T, H) = (T_c - T)^{\beta} \tilde{m}(H(T_c - T)^{-\beta\delta})$. On the other hand, one has exactly $m = 1 - 2\Sigma l n_l$, where $l = 1, 2, \ldots$ counts the total number of $\downarrow$ spins in a cluster, n_l is the number of clusters per site, and a 'cluster' is a group of $\downarrow$ spins surrounded by $\uparrow$ spins and otherwise quite arbitrarily defined. To give scaling for the magnetization, the cluster numbers should also follow a scaling homogeneity law (Binder 1976, equation (8)):

$$n_l(T, H) = l^{-2-y/\delta} \tilde{n}(H l^y, (T_c - T) l^z) \tag{2}$$

where δ is the usual critical exponent for the critical isotherm. (Here the prefactor in front of the scaling function $\tilde{n}$ is determined such that on the critical isotherm $m(T_c, H) = 2\Sigma l n_l(T_c, H) - 2\Sigma l n_l(T_c, 0)$ varies as $H^{1/\delta}$.) The quantity l^y can be regarded as the 'magnetization' of a cluster, i.e. as the excess number of spins compared to zero magnetization, to the average magnetization, or to some background magnetization (Kadanoff 1971, Stauffer *et al* 1971, Binder 1976, Kretschmer *et al* 1976). Since the spontaneous magnetization vanishes as $(T_c - T)^\beta$, one has $z = y/\beta\delta$. In general the main contribution to the singular parts of the various l-sums arises from l near $l_\xi \propto (T_c - T)^{-1/z} = (T_c - T)^{-\beta\delta/y}$, where l_ξ may correspond to cluster radii close to the correlation length ξ. Thus for any (large) exponent i we approximate $\Sigma l^i n_l \sim l_\xi^{i+1} n_{l_\xi}$.

For the new exponent y in equation (2) Binder derived rather generally an inequality (equation (29) of Binder 1976):

$$y \leqslant 1/(1 + 1/\delta) = \beta\delta/(2 - \alpha). \tag{3a}$$

(There is a misprint in Binder's equation (29) where $1 + 1/\delta$ has to be replaced by its reciprocal value.) With a particular simple assumption this inequality becomes an equality:

$$y = 1/(1 + 1/\delta). \tag{3b}$$

In the old Fisher model for critical point (Fisher 1967) or in percolation theory (dilute low temperature ferromagnets) one has $y = 1$; that choice is now excluded near T_c by the inequality (3a).

Now it is very easy to explain the difference between the second moment $S \propto (T_c - T)^{-\theta}$ and the susceptibility $\chi \propto (T_c - T)^{-\gamma}$:

$$S \propto \sum l^2 n_l \propto l_\xi^3 n_{l_\xi} \tag{4a}$$

$$\chi \propto \frac{\partial(\Sigma\, l n_l)}{\partial H} \propto \sum l^{1+y} n_l' \propto l_\xi^{2+y} n_{l_\xi}'. \tag{4b}$$

Thus the susceptibility no longer is given by the second moment; instead

$$S/\chi \propto l_\xi^{1-y} \propto (T_c - T)^{\beta\delta(1-1/y)}, \tag{5}$$

as the ratio of equations (4a,b) shows. With the simple choice (3b) we get

$$S/\chi \propto (T_c - T)^{-\beta}; \qquad \theta = \gamma + \beta, \tag{6a}$$

where the more general inequality (3a) gives

$$\theta \geqslant \gamma + \beta. \tag{6b}$$

In the two-dimensional Ising model, with $\beta = 1/8$ and $\gamma = 7/4$ we thus get

$$\theta \geqslant 1{\cdot}875, \tag{6c}$$

a result consistent with the $\theta = 1{\cdot}91 \pm 0{\cdot}01$ of Sykes and Gaunt (1976). Moreover, the simple choice (3b) for Binder's exponent y, with $\theta = 1{\cdot}875$, explains most of the difference between the exponents θ and γ. Therefore the Sykes and Gaunt data for two dimensions are roughly explained by Binder's cluster model.

Unfortunately this agreement is restricted to two dimensions. In general one has to be more careful in defining what a cluster is; so far this definition was open. In (site) precolation theory or for dilute low temperature ferromagnets it is appropriate to define a cluster as a set of occupied places or spins connected by nearest-neighbour bonds. For at $T=0$ even a single bond connecting two rather compact groups of spins as in the following diagram:

is forcing all the spins in the two groups to be parallel to each other; the left part cannot be oriented opposite to the right part at very low temperatures. (The dots in this diagram denote spins surrounded by non-magnetic atoms which are not shown.) But at higher temperatures such a single bond can quite easily be broken; and thus it may be more appropriate then to treat such a structure as two clusters. If instead of a dilute ferromagnet we look at a pure Ising model near its Curie temperature, then the dots of the diagram represent ↓ spins surrounded by ↑ spins which are not shown. Again the above structure may count as two clusters instead of one since at such high temperatures a single bond cannot keep the two rather large wings together (Binder 1976, figure 1). Thus it has been suggested for cluster-model descriptions of Curie points, that a 'cluster' or 'droplet' is in pure Ising models not just a group of parallel spins connected by nearest-neighbour exchange forces but is better regarded as a magnetization fluctuation, i.e. a region where the local magnetization density is larger than the average or background magnetization (Kadanoff 1971, Stauffer *et al* 1971, Kretschmer *et al* 1976).

Without such an appropriate cluster definition the clusters will percolate in three dimensions (Müller-Krumbhaar and Stoll 1976) before the Curie point is reached in a pure Ising model, and the critical behaviour will no longer be described by a scaling cluster model (equation (2)). Perhaps already in two dimensions the difference between $\theta = 1{\cdot}91$ and $\gamma+\beta = 1{\cdot}875$ indicates that clusters should not be defined simply as groups of nearest-neighbour-connected ↓ spins. For higher dimensions this difference in cluster definitions seems crucial even for the position of the phase transition. Thus in general one needs a still lacking 'cluster' definition which is as precise and practical as the usual (Sykes and Gaunt 1976) definition of clusters as sets of nearest-neighbour-connected spins but which instead does not count very loose structures as single clusters (Binder 1976).

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