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LETTER TO THE EDITOR

Coarse graining, Monte Carlo renormalisation, percolation threshold and critical temperature in the Ising model

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Abstract. Finite-size scaling suggests that the super-spins corresponding to large cells in a Monte Carlo renormalisation scheme form at $T = T_c$ an infinite network of connected down spins. Our finite-size scaling assumption, $M_b = f[(T-T_c)b^{1/\nu}]$ for the renormalised block spin magnetisation is tested by computer simulation for lattice sizes 128^3 and 256^3.

Clusters in Ising models or lattice gases are usually defined as groups of down spins connected by exchange forces J. If one approaches the Curie temperature T_c of the Ising magnet from below, and looks at the phase where most spins point up, then in general the percolation temperature $T_{\rm perc}$, where the down spins form for the first time an infinite connected network, does not coincide with T_c. For example, in the nearest-neighbour simple cubic Ising model, $T_{\rm perc}/T_c$ is about 0.96, with a magnetisation $M^{\rm perc}$ of about 0.6 at this percolation threshold (Müller-Krumbhaar 1974, Heermann and Stauffer 1981, Kertész *et al* 1983). Only in the modified cluster definition of Coniglio and Klein (1980), where bonds between up spins are formed randomly with probability $1-\exp(-2J/k_bT)$, is an infinite network of up spins connected by these additional bonds formed at the correct T_c where the magnetisation vanishes.

No such Coniglio-Klein bonds are taken into account in usual coarse graining theories (see for example Bruce and Wallace 1983) which work with a local magnetisation thought to come from averages over cells of linear dimension b. This averaging is done explicitly in some Monte Carlo renormalisation methods (Swendsen 1982, Pawley *et al* 1984, Jan *et al* 1983, Kalle 1984) where the spins in a cell of length b are replaced by a single superspin ± 1 having the orientation of the majority of the primary spins in that cell (with random tie breaking). Our question now is: Do these superspins percolate at the correct T_c, i.e. is an infinite network of down cells formed for the first time at $T_{\rm perc} = T_c$? We will argue that for finite cells this is not the case but that the positive difference $T_c - T_{\rm perc}(b)$ between the critical and the percolation temperature vanishes as $b^{-1/\nu}$ for $b \to \infty$.

We look at the renormalised magnetisation M_b of cells with b^d spins in a d-dimensional (hypercubic) lattice, $d < 4$, of linear dimension L, with $1 \ll b \ll L$. For $b = 1$, M_b simply gives the usual magnetisation of the primary spins. Our finite-size scaling assumption is

$$M_b = f[(T-T_c)b^{1/\nu}] \qquad (T \to T_c,\ b \to \infty) \tag{1}$$

where the correlation length $\xi \propto (T_c - T)^{-\nu}$ is assumed to be much smaller than L, but can be smaller or larger than b. We do not assume instead

$$M_b = b^{-\beta/\nu} f[(T-T_c)b^{1/\nu}] \tag{2}$$

where β is the critical exponent for the spontaneous magnetisation. Equation (2) would be correct (Fisher 1971, Landau 1976, Binder 1981) for the usual magnetisation measured in a system of size b; then $b=\infty$ is the desired thermodynamic limit.

In our case, however, $b=1$ and not $b=\infty$ corresponds to the usual magnetisation, whereas $M_b \to 1$ for $b \to \infty$ at fixed T below T_c. For in a large enough cell below T_c, $\xi \ll b$, the relative magnetisation fluctuations are negligible, the majority of spins point upwards, and thus $M_b = 1$. Figure 1 shows qualitatively the difference between equation (1) for our renormalised magnetisation M_b and equation (2) for the usual magnetisation in a system of finite size b; if $b=1$, in the latter case the 'magnetisation' of the single-spin system is always ± 1. Our renormalised magnetisation M_b of equation (1) therefore is not analogous to the magnetisation in small systems, equation (2). Instead it corresponds to the probability R of percolative systems (Reynolds *et al* 1980, Stauffer 1985) to have a cluster connecting top and bottom in a cell of size b; this probability R also approaches zero or unity for large enough cells and follows the analogue of equation (1).

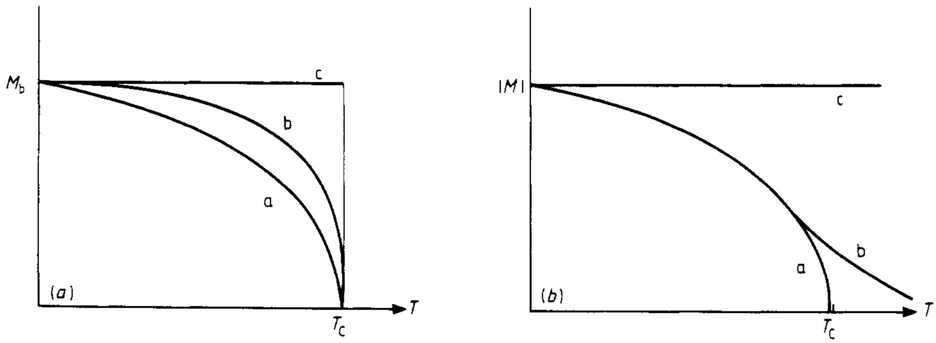

Figure 1. Qualitative comparison of renormalised magnetisation due to cells of size b in a much larger system of size L (a) equation (1) ((a, $b=1$; b, b large; c, $b=\infty$) and of the usual magnetisation in a finite system of size L (b) equation (2)) (a, $L=\infty$; b, L large; c, $L=1$).

For the unrenormalised primary spins ($b=1$) the percolation threshold is reached at $T = T_{\text{perc}}(b=1)$ below T_c, with a positive magnetisation $M = M_{b=1}^{\text{perc}}$; for the clusters formed by upward oriented neighbouring b cells the percolation threshold is at $T_{\text{perc}}(b)$ and M_b^{perc}. Experience with dynamic renormalisation (Jan *et al* 1983, Kalle 1984) warns against assuming $M_{b=1}^{\text{perc}} = M_b^{\text{perc}}$ and suggest instead, similar to percolation (Reynolds *et al* 1980):

$$M_b^{\text{perc}} = M_{b'}^{\text{perc}} \quad (b \text{ and } b' \gg 1). \tag{3}$$

Equations (1) and (3) give

$$[T_c - T_{\text{perc}}(b)]/[T_c - T_{\text{perc}}(b')] = (b/b')^{-1/\nu} \tag{4}$$

for large enough cells, and thus

$$T_c - T_{\text{perc}}(b) \propto b^{-1/\nu} \qquad (b \to \infty). \tag{5}$$

The reason behind equations (3)-(5) is the similarity of block spins and primary spins on which scaling and real space renormalisation are based: The correlations between primary spins and between cells are about the same apart from factors of order unity, provided the distance is measured in terms of the correlation length ξ. Therefore the concentration M^{perc} of up cells at the percolation threshold T_{perc} is the same, whether the cells are large or very large.

Direct Monte Carlo evaluation of $T_{\text{perc}}(b)$ might be difficult for large b and should be combined (Binder, private communication) with a detailed comparison of cluster size distributions for the renormalised superspins and the Coniglio–Klein clusters of primary spins. As a first step, we test here the underlying scaling assumption (1) on a CDC Cyber 205 vector computer. To satisfy $1 \ll b \ll L$ our system has to be large. We thus made up to 10^5 Monte Carlo steps per spin for $L = 128$ in a simple cubic lattice between $0.82 T_c$ and $0.999 T_c$, as well as shorter runs for $L = 256$, using Kalle's program. Our equilibrium results (at $0.999 T_c$ extrapolated to $L = \infty$) are shown in figure 2. There $b = 1$ slightly deviates from the scaling assumption (1), as expected, but larger b confirm the similarity rule (1).

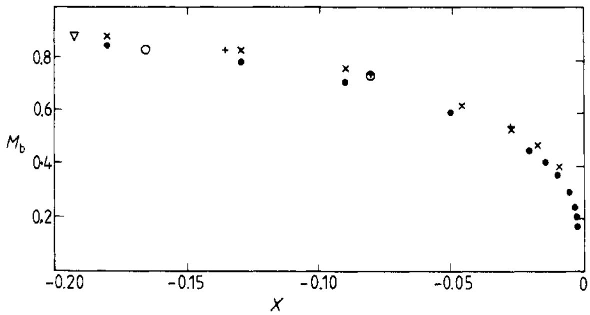

Figure 2. Variation of the renormalised magnetisations M_b with $X \equiv b^{1/\nu}(T - T_c)/T_c$. Our Monte Carlo data ($128^3$ and 256^3 simple cubic lattices) for $b = 4, 8, \ldots$ as listed in the figure follow roughly the same curve and thus confirm equation (1). The factor $b^{1/\nu}$ by which equations (1) and (2) differ varies by roughly a factor 2 between $b = 4$ and $b = 16$; thus our data contradict equation (2). (●, $b = 1$; ×, $b = 4$; +, $b = 8$; ○, $b = 16$; ▽, $b = 32$).

Thus we see little reason to doubt that the percolation threshold for clusters of Ising superspins in real space renormalisation converges to the desired critical temperature T_c if the cell size b for these superspins goes to infinity. Our result justifies droplet models based on coarse-grained order parameters near T_c and makes feasible future studies of cluster size distributions.

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