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Critical droplet for the three-dimensional Ising model

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Abstract. The droplet model is investigated in the critical region by Monte Carlo simulation with a novel definition of droplets. The size distribution of droplets of size l is found to be $n_l \approx l^{-\tau} \exp[-(K - K_c)^\mu s l^\zeta]$, where $(K - K_c)^\mu$ stands for the surface tension with K denoting the reduced temperature, and $s l^\zeta$ for the surface area; the numerical constants are given by $\tau = 2.21$, $\mu = 1.0$ and $\zeta = 0.78$ for the simple cubic lattice. The droplet is prescribed properly by taking account of the density correlation between the centre and the perimeter, which has no singularity at the percolation point.

The droplet model has contributed much to our understanding of phase transitions, particularly of nucleation, the metastable phase and the coexistent phase line (Langer 1967, Fisher 1967). This phenomenological concept has been widely accepted as being effective in the low temperature region, where a droplet forms to optimise the surface energy. Near criticality, however, the functional form of the surface free energy is not clear owing to poor knowledge of the entropy term.

In the critical region, the size distribution of droplets proposed by Fisher (1967) has been examined directly by computer simulations for the Ising spin lattices (Müller-Krumbhaar and Stoll 1967, Stoll *et al* 1976). According to these simulations, there appears a percolation singularity, which makes difficult a simple interpretation of the droplet in terms of clustering of particles (Müller-Krumbhaar 1974). However, from such a correlated percolation problem, various model theories have developed: the Coniglio-Klein model (1980, Kertész *et al* 1983) based on the Kasteleyn-Fortuin technique (1969), polychromatic percolation in supercooled water (Stanley 1979) and the liquid-like cell percolation in liquid-glass transitions (Cohen and Grest 1979).

In the present paper, we reconsider Fisher's droplet model by means of Monte Carlo (MC) simulation for an Ising lattice, where a phenomenological scaling theory is utilised by assuming the free energy of a droplet to consist of the bulk term and the surface one. On analysing the simulation data, we notice the size of the density fluctuation which should be less than the correlation length ξ . This condition is very important in prescribing the connectedness of a pair of particles in a cluster. A careful criterion for the connectedness allows us to get over the difficulty of the percolation singularity, since the correlation length is not singular at the percolation point (Nagao 1980). The cluster thus well defined will be shown to have the features of droplets, particularly near criticality.

Our computer simulation is described below in detail. For the Ising system with periodic boundary condition, we take the Hamiltonian to be

$$H = -J \sum_{\langle i,j \rangle} \mu_i \mu_j, \quad \mu_i = \pm 1, \tag{1}$$

with $\langle i, j \rangle$ denoting a nearest-neighbour pair in a simple cubic lattice. In the simulation, we generate about 7×10^3 steps/spin at temperatures $\varepsilon = 0.04, 0.075, 0.10$ and 0.15 with $\varepsilon = 1 - T/T_c$ and 6×10^3 at $\varepsilon = 0.20$, where the total number N of spins is taken to be $30 \times 30 \times 30$. On the lattice site, we randomly distribute up spins, whose density is made equal to that expected for the system in equilibrium at the temperature of the experiment. The first MC steps, ranging from several hundred to a few thousand, are discarded until the equilibrium state is reached.

In a Markovian chain of the spin configuration generated by the conventional method (Glauber dynamics), the size, the surface area and the radius of a droplet are defined as follows.

(i) For a given configuration of spins, we number the up-spin sites in the order in which the number of the nearest neighbours having up spin decreases; we do this randomly if two or more sites have the same number of nearest neighbours with up spin. This numbering is illustrated in figure 1.

(ii) Of the up-spin sites thus numbered, we start with the first one (1 in figure 1(b)), and then visit the nearest-neighbouring sites (5, 8, 12, $\bar{1}$) at the first step, the next-nearest-neighbouring ones (3, 9, 14, $\bar{1}-\bar{5}$) at the second step and so on.

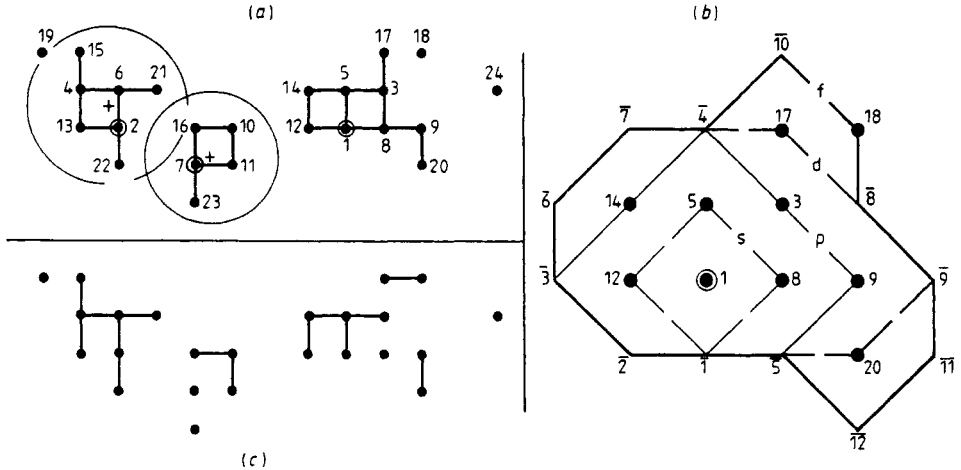


Figure 1. Prescription of droplets. A snapshot of the configuration of the spins taken at the temperature $0.960 T_c$ in a square lattice. The equilibrium density $\langle \rho \rangle_T$ of the up spin is 0.092 for the total lattice. A dot (●) denotes an up-spin site; no down-spin site is marked. (a) Droplets (connected dots ●—●) prescribed by the author's criterion. Dots stand for the original configuration of up-spin sites. Labelling with numbers and symbols is done for droplet construction: ● denotes the starting point, + the centre and a full circle the radius R for each droplet. (b) Droplet construction. The density of the dots in each shell (labelled $s-d$) does not become less than $\langle \rho \rangle_T$ until in the f shell; the size l of the droplet is given by the total number of dots within the d shell; all the surface sites S are only in the f shell; $l=9, S=13, R=2.54$. For a dot (18), $l=1, S=4, R=0.50$. (c) Droplets (connected dots ●—●) based on the Coniglio-Klein criterion.

(iii) If we visit a down spin ($\bar{1}-\bar{12}$) in the above process, we stay there ($\bar{1}-\bar{9}$) in the next step. Thus we have a concentric shell (labelled by s-f) of the sites at every step with the starting point as the centre.

(iv) We stop stepping when the up-spin density $\langle \rho(r) \rangle$, which is the average of the density $\rho(r)$ over all the sites (in the r th shell) visited at the r th step, becomes less than the thermal average density $\langle \rho \rangle_T$ for the total system.

(v) The size l of droplets is defined by the total number of up spins (at 1 and in s-d shells) which have been visited up to the last step, the number $S(l)$ of the surface sites by the number of sites (in the f shell) just visited at the last step, and the radius $R(l)$ by the maximum distance between the centre (labelled by +) and an up spin in the droplet. (For the radius, we add one-half of the lattice constant to the maximum distance. Circles with the above radii are depicted in figure 1(a).)

(vi) Returning to the beginning, we choose the up-spin site of the earliest ordinal number (2) among the remaining up-spin sites and repeat the same procedures as before and so on. The procedure continues until the sites of interest are exhausted (figure 1(a)). Here the up spins counted already in the preceding procedures are regarded as down spins to prevent double counting.

The number $S(l)$ of the surface sites thus obtained is plotted in figure 2 as a function of l , which may be fitted to

$$S(l) \sim l^\zeta \tag{2}$$

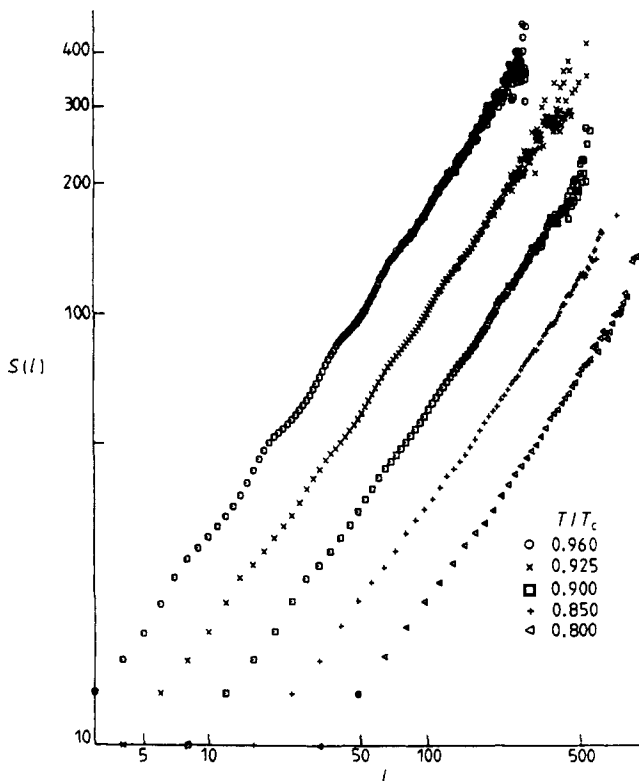


Figure 2. Number $S(l)$ of surface sites as a function of size l for droplets. Index ζ equals 0.783 (O); 0.775 (x); 0.765 (□); 0.753 (+); 0.768 (Δ). Marks x are shifted by $\log 2$ on l axis; □ by $2 \log 2$; + by $3 \log 2$; Δ by $4 \log 2$.

with ζ denoting the slope of the lines. The size of droplets as a function of the radius R has also proved to be fitted to

$$l \sim R^{D'} \tag{3}$$

with a fractal dimension D' , as can be seen in figure 3.

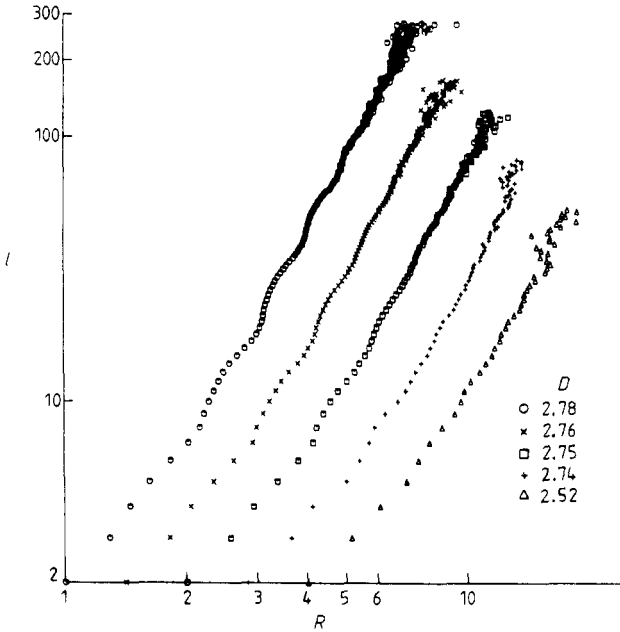


Figure 3. Size $l(R)$ as a function of radius for droplets. For the experimental temperatures, refer to figure 2. Marks \times are shifted by $0.5 \log 2$ on the R axis; \square by $\log 2$; $+$ by $1.5 \log 2$; \triangle by $2 \log 2$.

Let us refer to a phenomenological scaling theory before going into an examination of the size distribution of droplets. In the critical region, the free energy density f follows the scaling law

$$f(\varepsilon, h) = L^{-d} f(\varepsilon L^{1/\nu}, h L^D), \tag{4}$$

where h is the field, L the scaling factor, d the Euclidean dimension, $D \equiv d - \beta/\nu$ with β and ν the familiar critical indices and f is a scaling function. For a partial system characterised by length R , the free energy density is then transformed into

$$f(\varepsilon, h, R) = L^{-d} f(\varepsilon L^{1/\nu}, h L^D, R L^{-1}) = R^{-d} f(\varepsilon R^{1/\nu D}, h R^D), \tag{5}$$

if the system has a dilational symmetry for the scaling. Let us assume $R^D \sim l$ with R the radius and D the fractal dimension for droplets, though equation (3) does not offer sufficient evidence to support this assumption. Then we have

$$f(\varepsilon, h, l) = l^{-d/D} f(\varepsilon l^{1/\nu D}, h l). \tag{6}$$

The size distribution n_l may be obtained from the partial derivative of the function f with respect to l :

$$n_l \sim \partial f / \partial l \sim l^{-(d/D)-1} n(\varepsilon l^{1/\nu D}, h l), \tag{7}$$

which is identified with Fisher's results if $n(x, y) \sim \exp(ax + by)$. The scaling relation (7) does not change on replacing $\varepsilon l^{1/\nu D}$ by $\varepsilon^\mu l^\zeta$, provided that

$$\mu/\zeta = \nu D. \tag{8}$$

However, if the surface area $S(l)$ is of the form sl^ζ with s a proportional constant, the surface tension $\gamma(\varepsilon)$ must be of the form

$$\gamma(\varepsilon) \approx (K - K_c)^\mu, \tag{9}$$

where K denotes $J/k_B T$ and $K_c = 0.2217$ (Pawley *et al* 1984). Dropping the field term, we predict the distribution function in the following form,

$$n_l(\varepsilon) \sim l^{-\tau} \exp[-\gamma(\varepsilon)S(l)], \tag{10}$$

with $\tau \equiv (d/D) + 1$, because each droplet has no density correlation between the centre and the perimeter and is thus isolated from others in the average density $\langle \rho \rangle_T$ of spins.

The distribution function predicted above proves relevant according to our simulation results. This is shown in figure 4. The index μ can be determined from the slope of the curves for $-\log(n_l l^\tau)$ against l^ζ with the use of (2) and (9). They are tabulated in table 1. There exist some deviations of our simulation data from the scaling law (10), for both regions of small and large values of l . In the region of small l , the deviation is due to the size effect, as pointed out by Kalos *et al* (1978) who proved failure of the scaling to occur for $l \leq 10$. It seems that the oscillations in n_l reflect that the up spins (one spin occupies a finite cell) closely pack into the concentric shells to form a droplet. For large droplets, on the other hand, the size can exceed the correlation volume ξ^d . Since larger droplets occur less frequently, we need many more MC steps to establish the size distribution for large l .

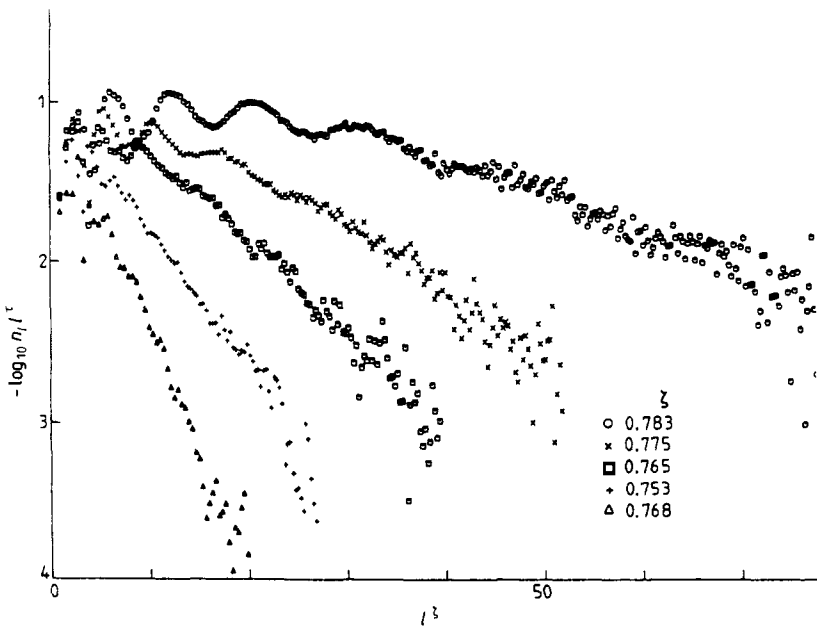


Figure 4. Size distribution n_l against number l^ζ of surface sites for droplets ($n_l \sim a(\varepsilon)l^{-\tau} \exp -(K - K_c)^\mu s l^\zeta$). K is the reduced temperature defined by $J/k_B T$. Lines are drawn for the determination of the indices μ . The amplitude $a(0) = 0.88$, $\tau = 2.21$.

Table 1. Scaling indices for size distribution and for characteristic features of droplets. m is the spontaneous magnetisation measured in our simulation, m_s the expected one from series expansions (Essam and Fisher 1963). $m_s = -1.57(1 - T/T_c)^{0.3125}$.

$1 - T/T_c$	μ	ζ/μ	m/m_s	d	D	$1/\nu D$	$(d-1)/D$	μ^a
0.040	0.99	0.791	0.978	2	1.875	0.553	0.553	1.000
0.075	1.00	0.775	0.962	3	2.50 ^b	0.63 ^b	0.80 ^b	1.26 ^b
0.100	0.99	0.773	0.951	4	3.000	0.667	1.000	1.500
0.150	1.03	0.731	0.927					
0.200	—	—	0.906					

^a $\mu = \nu(d-1)$ Widom (1972).

^b Index ν is given by Pawley *et al* (1984) or by George and Rehr (1984).

At this point we mention Widom (1972), who proposed that temperature dependence of the surface tension is given by $\gamma(\varepsilon) = (K - K_c)^{\nu(d-1)}$ for a macroscopic interface ($l \gg \xi^d$). The above expression proves equivalent to putting

$$\mu = \nu(d-1) \quad (11)$$

in (9). This expression leads us to an assumption of

$$S(l) \sim (l^{1/D})^{(d-1)}, \quad (12)$$

that is, $S(R) \sim R^{(d-1)}$ with R the radius. The numerical values of the indices appearing in (6)-(12) are tabulated in table 1 for dimensions $d = 2, 3$ and 4 , in comparison with our experimental ones.

In a square Ising lattice, the above point of view explains why a good result has been obtained by Fisher's model: no difference is verified between the models (7) and (12) owing to the coincidence between $1/\nu D$ and $(d-1)/D$ or to that between $d-1$ and $\nu(d-1)$.

Critical droplets, whose ranges are smaller than the correlation length ξ , have the same scaling properties as the correlation droplet with the range ξ . This is due to the similarity in the renormalisation of their thermal fluctuation as given in (4) and (5).

Thus each critical droplet will be distinct from the medium of spins in the average over its fluctuation. We note here that for each droplet the fluctuation of spins lying on the perimeter has been taken into account at each MC step. Accordingly the boundaries of our droplets have appeared only through the average over the fluctuations. Besides, these droplets have been shown to follow the scaling law, as the result of averaging over the ensemble of our MC simulation.

The percolative connectedness is very sensitive to thermal fluctuation, even the smallest (a string can be broken by a spin flip). It is then inadequate for the prescription of critical droplets. The droplets based on the Coniglio-Klein criterion (see figure 1(c)) are clusters consisting of bonds with a specific probability among the up spins at each MC step. Such bonds would work to cut off the other bonds in the region of dense up-spins so that a cluster might be the critical droplet.

Next we discuss the indices obtained in this experiment. The index ζ asymptotically approaches 0.80 as ε approaches 0 and nearly equals $(d-1)/D = 0.780$. The index μ is equal to 1.00 and close to Widom's 1.26 provided that this theory is applicable to a finite size droplet. The ratio μ/ζ differs from νD by 20%. This figure is thought of as the degree of the deviations of our results from the familiar critical indices. It is not clear, however, whether it is attributable to our system being finite and/or being

away from criticality. Our result for the fractal dimensionality $D' \approx 2.76$ is larger than $D = d - \beta/\nu = 2.50$. Moreover, the following may be worth noting. The radius in (3) is given by the maximum length of a straight line extending from the centre to the perimeter for a droplet, while the number of steps is the scale of length in the droplet construction. This duality could be serious in estimating numerical value of D' for small droplets. It is because the number of steps cannot be smaller than the length of a straight line between any two sites.

Note added in proof. At the temperature $0.980 T_c$, no droplet has proved to percolate infinitely in 8900 MC steps/spin for $40 \times 40 \times 40$ system: the values of the indices ζ , μ and D appear to equal those in the text, while all the evaluation has not been finished. A study of a metastable state is in progress.

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