Bulk, surface and hull fractal dimension of critical Ising clusters in d=2

1989 J. Phys. A: Math. Gen. 22 L445

(http://iopscience.iop.org/0305-4470/22/10/005)

J. Phys. A: Math. Gen. **22** (1989) L445–L451. Printed in the UK

LETTER TO THE EDITOR

Bulk, surface and hull fractal dimension of critical Ising clusters in $d = 2$

Carlo Vanderzande† and Attilio L Stella‡

† Limburgs Universitair Centrum, 3610 Diepenbeek, Belgium
‡ Dipartimento di Fisica dell'Universita and CISM, 35131 Padova, Italy

Received 21 February 1989, in final form 23 February 1989

Abstract. We present accurate numerical calculations of the fractal dimension $\bar{d}$ and surface dimension $\bar{d}_s$ of the critical Ising cluster, in $d = 2$. Our results clearly support the values $\bar{d} = \frac{187}{96}$, $\bar{d}_s = \frac{5}{6}$ which are consistent with Ising clusters being described by tricritical $q = 1$ Potts model exponents. From this, the hull dimension $\bar{d}_H$ of critical Ising clusters is found to be $\bar{d}_H = \frac{11}{8}$, consistent with numerical work of other authors.

The study of clusters of sites with, e.g., spin up in the Ising model, originating in the droplet picture of critical behaviour (Fisher 1967) has been an active field in the last 20 years. This interest is mainly caused by the fact that the clusters could give a description of critical behaviour in terms of geometrical properties (Binder 1976).

If a site with spin up (down) is considered as being occupied (unoccupied), the problem of Ising clusters can be translated into a problem of (Ising) correlated site percolation. In this way, many concepts from percolation, such as cluster numbers, percolative free energy, etc, can be used also in the study of Ising clusters. For example we can define n_s (T, g) as the (thermal) average number of s clusters (per site) when the Ising model is at temperature T and in a magnetic field g. Besides these finite clusters, one infinite cluster may also be present in the model. As in the case of ordinary percolation, one may then for example look for the fractal properties of this infinite cluster.

Let us first briefly review what is known about the Ising clusters from exact results (Coniglio *et al* 1977). We will limit ourselves here to the two-dimensional case. For $K = J/kT \geqslant K_c$ there exists one infinite cluster of up spins for all $h = g/kT > 0$, which is a two-dimensional object (K_c is the critical value of the two-dimensional Ising model, e.g. $\sinh^2 K_c = 1$ on the square lattice). Such a cluster also exists for all $K < K_c$, $h > h_0(K)$ where the function $h_0(K)$ is not completely known. For $K \to 0$, h_0 approaches a value determined by the site percolation threshold p_c (for uncorrelated percolation), given by $\exp(h_0(0))/2 \cosh h_0(0) = p_c$. Finally, it was recently shown (Stella and Vanderzande 1988) that for $K \to K_c^-$, $h_0(K)$ should behave as

$$h_0(K) \sim (K_c - K)^{15/8}. \tag{1}$$

Precisely at $K = K_c$, $h = 0$ there exists one infinite cluster of up (down) spins which is a fractal. We will refer to this cluster as the incipient infinite Ising cluster (I^{3}C for short). In the present letter we determine the fractal dimension of the I^{3}C. Moreover, we study the fractal dimension of critical Ising clusters in a semi-infinite geometry. As shown below, on the boundary the cluster fractal dimension, $\bar{d}_s$, is simply related to the percolative magnetic surface exponent y'_H of the Ising model. As in other problems of two-dimensional critical phenomena, consideration of such surface exponents can be an extremely important and sensible check for the appropriate classification within conformal invariance schemes. In the case of Ising clusters at Onsager's critical point, such a classification has recently been obtained by the present authors. The work presented here leads to a further confirmation and derives some new consequences of these results.

The approach we take combines Monte Carlo calculations in finite systems with a finite-size scaling analysis (Barber 1983, Nightingale 1982). This technique was recently applied to the case of ordinary percolation (Vanderzande 1988). Let us define a percolative free energy for the cluster numbers $n_s(K, h)$ as

$$f(K, h, H) = \sum_s n_s(K, h) \exp(-sH). \tag{2}$$

Here H is a 'ghost' field, similar to the one used in ordinary percolation (see e.g. Essam 1980). From (2), a *percolative* susceptibility $\chi_{\mathrm{P}}(K, h)$ can be defined as (for $H = 0$)

$$\chi_{\mathrm{P}}(K, h) = \frac{\partial^2 f}{\partial H^2}\bigg|_{H=0} = \sum_s s^2 n_s(K, h). \tag{3}$$

In the neighbourhood of the Ising critical point $K = K_c$, $H = h = 0$, f obeys a scaling law of the form

$$f(K, h, H) \sim b^{-2} f(b^{y_t} K, b^{y_h} h, b^{y_H} H). \tag{4}$$

Let us now consider this problem in a finite geometry, e.g. in a square of $L \times L$ sites. Then, the scaling law (4) is modified into

$$f(K, h, H, L) \sim b^{-2} f(b^{y_t} K, b^{y_h} h, b^{y_H} H, b^{-1} L). \tag{5}$$

As a consequence, at the Ising critical point the susceptibility χ_{P} in a finite system is expected to grow as

$$\chi_{\mathrm{P}}(K_c, h = 0, L) \sim L^{-2+2y_H} \tag{6}$$

with the system size.

As in ordinary percolation (Stanley 1977), y_H can be interpreted as the fractal dimension of the $\mathrm{I}^3\mathrm{C}$. To see this, define $P(K, h)$ as the probability that a given site belongs to the infinite cluster of up spins. The probability that a spin is up is given by $\frac{1}{2}(m(K, h) + 1)$ where $m(K, h)$ is the magnetisation of the Ising model. If the spin is up it is in the infinite cluster with probability $P(K, h)$, and in a finite cluster with probability $\Sigma_s sn_s(K, h)$; thus we have

$$P(K, h) = \tfrac{1}{2}(m(K, h) + 1) - \sum_s sn_s(K, h). \tag{7}$$

Along the line $h = 0$, $m(K, h)$ will behave as

$$m(K, h) \sim (K - K_c)^{(2-y_h)/y_t = 1/8} \qquad K > K_c \tag{8a}$$

and from (4) the singular part of $\Sigma_s sn_s(K, H)$ behaves as

$$\sum_s sn_s(K, h) \sim (K - K_c)^{(2-y_H)/y_t} \qquad K > K_c. \tag{8b}$$

As we will see later $y_H > y_h$ and thus we finally obtain that

$$P(K, h = 0) \sim (K - K_c)^{(2-y_H)/y_t} \qquad K > K_c. \tag{9}$$

If one also defines ξ, a correlation length†, which for $h=0$ behaves as

$$\xi(K,0) \sim |K-K_c|^{-\nu} \tag{10}$$

with $\nu = 1/y_t$, (9) and (10) give

$$P(K>K_c,0) \sim \xi(K,0)^{y_H-2}. \tag{11}$$

If one remembers that the relation between the density ρ of a fractal and a typical length scale L defines the fractal dimension $\bar{d}$ as (Mandelbrot 1982, Pietronero and Tosatti 1986)

$$\rho \sim L^{\bar{d}-D} \tag{12}$$

(where D is the dimension of the Euclidean space in which the fractal is embedded), then we can interpret y_H as the fractal dimension of the $\mathrm{I}^3\mathrm{C}$, from (9), (11) and (12).

To summarise, if one calculates $\chi_p(K_c, 0, L)$ in systems of different size L, one can obtain from (6) $\bar{d} = y_H$ of the $\mathrm{I}^3\mathrm{C}$.

As in the case of ordinary percolation (Vanderzande 1988) we are also interested in the surface fractal dimensions, $\bar{d}_s$ of the $\mathrm{I}^3\mathrm{C}$. This dimension can be found if one considers a semi-infinite system. The fractal dimension of the sites in the $\mathrm{I}^3\mathrm{C}$ and on the surface is then called the surface fractal dimension $\bar{d}_s$. Once more this $\bar{d}_s$ is related to a critical exponent y'_H which describes the percolative properties of Ising clusters in a semi-infinite geometry. As in the case of ordinary percolation (De'Bell 1980), we can now define cluster numbers $n_{s,s_0}(K,h)$ which give the average numbers of clusters (per site) containing s sites, s_0 of which are at the surface. From this one can define a free energy

$$f(K,h,H,H_s) = \sum_{s,s_0} n_{s,s_0}(K,h)\exp(-sH - s_0H_s) \tag{13}$$

(H_s is a surface ghost field) and a surface percolative susceptibility $\chi_{p,s}$

$$\chi_{p,s}(K,h) = \left.\frac{\partial^2 f}{\partial H\,\partial H_s}\right|_{H=H_s=0} = \sum_{s,s_0} n_{s,s_0}(K,h)ss_0. \tag{14}$$

In the surface geometry, (5) is modified into

$$f(K,h,H,H_s,L) \sim b^{-2} f(b^{y_t}K, b^{y_h}h, b^{y_H}H, b^{y'_H}H_s, b^{-1}L) \tag{15}$$

which gives for $\chi_{p,s}$ at the Ising critical point

$$\chi_{p,s}(K_c,0,L) \sim L^{-2+y_H+y'_H}. \tag{16}$$

The argument given earlier in this letter can now be extended to show $\bar{d}_s = y'_H$ (Vanderzande 1988).

We have determined y_H and y'_H in the following way. We perform Monte Carlo calculations of an Ising model of $L\times L$ sites at criticality. We take periodic boundary conditions in one direction and free boundary conditions in the other, thus creating a free surface. After equilibrium has been reached, we count for each spin configuration the cluster numbers n_{s,s_0} using standard cluster counting techniques (Stauffer 1985).

After averaging n_{s,s_0} over a great number of spin configurations, the susceptibility $\chi_p(K_c, 0, L)$ and surface susceptibility $\chi_{p,s}(K_c, 0, L)$ are calculated from (3), respectively (14), and fitted to (6) and (16) to obtain y_H and y'_H.

† Such a correlation length can e.g. be obtained from the percolative correlation function $g(r)$, which gives the probability that a site a distance r from an occupied site is also occupied and belongs to the same cluster.

We performed calculations for systems with $L = 4, 6, 8, \ldots, 24, 26, 30$ and 36. For the largest system size, up to 1.25×10^6 MC steps/spin were performed. Also for $L \leq 26$, two independent runs were made. Errors were estimated from fluctuations in subresults. Before discussing our results we would like to make a remark on the boundary conditions. It can be admitted that for the calculation of χ_p, periodic boundary conditions in two directions at first sight might have been a better choice. We believe, however, that for the large systems considered here boundary conditions are not too important in determining bulk properties. As the calculations are rather time consuming, we choose to determine in one calculation both bulk and surface susceptibility.

Figure 1(a) shows the quantity $\log \chi_p$ plotted against $\log L$. As can be seen, they lie on a straight line, whose slope gives $y_H = 1.936(\pm 0.009)$. The results on $\chi_{p,s}$ (figure 1(b)) give

$$\chi_{p,s}(K_c, 0, L) \sim L^{0.778(\pm 0.007)} \tag{17}$$

from which, using the above result on y_H, we find $y'_H = 0.842(\pm 0.008)$.

Our result for $\bar{d} = y_H$ is consistent with a previous, less accurate determination (Cambier and Nauenberg 1986) which gave $\bar{d} = 1.90(\pm 0.06)$. Furthermore a result obtained by series enumerations (Sykes and Gaunt 1976) gave the exponent $\gamma = 1.91(\pm 0.01)$, which is related to y_H by $\gamma = (-2 + 2y_H)/y_t$. From this we obtain $y_H = 1.95$. In order to obtain this result we had to use $y_t = 1$ (Coniglio and Klein 1980, Stella and Vanderzande 1988). Our calculation has the advantage of giving a direct determination of y_H alone.

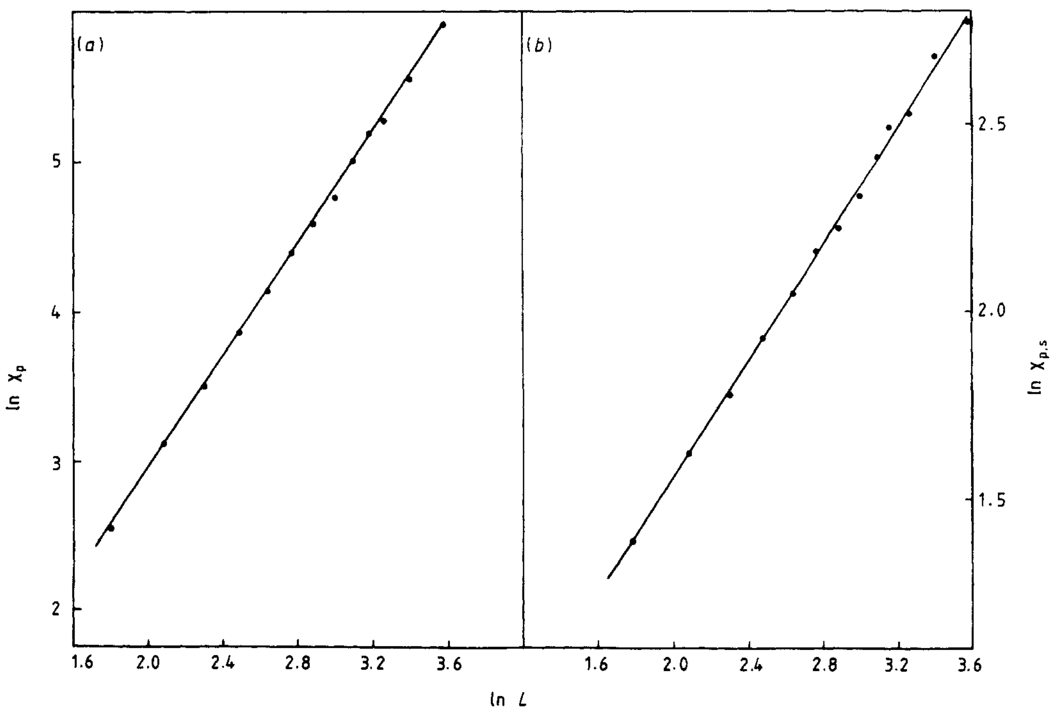

Figure 1. Logarithm of bulk percolative susceptibility χ_p (a) and surface percolative susceptibility $\chi_{p,s}$ (b) at the Ising model critical point, plotted against logarithm of system size L. The straight lines give least-squares fits.

Our results clearly contradict a conjecture (Suzuki 1983) according to which $y_H = \bar{d} = \frac{15}{8} = 1.875$.

On the other hand our results are consistent with a recent result of the present authors (Stella and Vanderzande 1988) according to which the critical Ising point is a tricritical point for correlated percolation. Then, by studying the $q \to 1$ limit of the Potts lattice gas, and using results from conformal invariance (Stella and Vanderzande 1988) it can be argued that the exponents describing the Ising cluster are those of the tricritical $q \to 1$ Potts model (such a relation was first proposed by Temesvári and Herényi (1984) on a more conjectural basis). In that case we would have $y_H = \frac{187}{96} = 1.947\ldots$ (Nienhuis 1987), a value which is clearly supported by our results.

Our determination of $y'_H = \bar{d}_s$ is the first we know of. Extending the result of Stella and Vanderzande (1988) to the case of the surface fractal dimension, one concludes that y'_H should be given by one of the surface magnetic exponents of the tricritical $q = 1$ Potts model.

Unfortunately, within conformal invariance alone there is no definite *a priori* solution to the question of what these exponents should be. If one extends a result for the critical branch of the Potts model (Cardy 1984) to the tricritical branch one obtains (Vanderzande and Stella 1987)

$$y'_H = u \tag{18}$$

where $u = (2/\pi)\cos^{-1}\sqrt{q}/2$, and for the tricritical branch of the Potts model one should take $-1 \leqslant u \leqslant 0$ (Wu 1982).

For $q = 2$, the tricritical Ising model, one obtains in this way $y'_H = -\frac{1}{2}$. This result is in agreement with an independent determination by Cardy (1986) and with numerical results (Balbão and Drugowich de Felicio 1987).

For the case of interest here, $q = 1$, we obtain $y'_H = -\frac{2}{3}$. This result is clearly in contradiction with our numerical data, but also with the interpretation of y'_H as a surface fractal dimension, which of course should be positive.

At a tricritical point we expect two magnetic surface exponents and thus a surface exponent like we find would not necessarily contradict the identification of the Ising clusters with the tricritical $q = 1$ Potts model.

We can obtain with some plausible arguments a lower bound on y'_H. From the physics of the problem and also from our result on $\bar{d}$ it is clear that the $\mathrm{I^3C}$ is a more compact fractal than the incipient infinite cluster ($\mathrm{I^2C}$) in the percolation problem (remember that in that case, $\bar{d} = \frac{91}{48} < \frac{187}{96}$). One thus also expects that the surface fractal dimension of the $\mathrm{I^3C}$ is bigger than that of the $\mathrm{I^2C}$, which equals $\frac{2}{3}$ (Cardy 1984, Vanderzande 1988). Thus we obtain $y'_H \geqslant \frac{2}{3}$, consistent with our numerical result.

Using results from conformal invariance (see Cardy 1987 for a review) we can give a conjecture for y'_H. The tricritical point of the $q = 1$ Potts model is described by a non-unitary conformal field theory with central charge $c = \frac{1}{2}$. In that case possible surface exponents are determined from the Kac formula and are given by $1 - \Delta_{p,q}$ where

$$\Delta_{p,q} = \frac{(4p-3q)^2 - 1}{48} \tag{19}$$

with p and q arbitrary integers. Taking $\Delta_{3,3}$ we obtain $y'_H = 1 - \Delta_{3,3} = \frac{5}{6} = 0.833\ldots$, in good agreement with our result. Taking our conjectured values for y_H and y'_H in (16) we obtain

$$\chi_{\mathrm{p,s}}(K_c, 0, L) \sim L^{75/96 = 0.781}$$

which is almost exactly the numerical result in (16).

Thus, if the critical Ising clusters are indeed described by a tricritical $q=1$ Potts model, this model seems to have one relevant ($\frac{5}{6}$) and one irrelevant ($-\frac{2}{3}$) surface magnetic exponent. The numerical results of Balbão and Drugowich de Felicio (1987) who worked on the Blume-Capel model, which is thought to be in the same universality class as the tricritical Ising model, indicate, however, that for $q=2$, there is no relevant surface magnetic exponent for the tricritical point in the Potts model. It may be that in this case, unitarity (Friedan *et al* 1984) forbids some exponents to appear in the theory. This may be an interesting subject for further study.

The numerical calculations presented above clearly support the idea that critical Ising clusters are described by tricritical $q=1$ Potts model exponents. This equivalence allows us to determine one more fractal dimension of the Ising clusters, namely the dimension of the hull, $\bar{d}_{\mathrm{H}}$ (here H should not be confused with any of the magnetic fields introduced above). The hull of a cluster is defined as the set of nearest-neighbour sites of the cluster, for which a path to infinity exists which does not cross the cluster.

The fractal dimension of the hull for arbitrary values of q in the q-state Potts model was calculated using Coulomb gas methods by Saleur and Duplantier (1987). In the case of the tricritical $q=1$ Potts model their result can be seen to lead to

$$\bar{d}_{\mathrm{H}}=\tfrac{11}{8}(=1.375). \tag{20}$$

Numerical evidence that this is indeed the hull dimension of the $\mathrm{I}^3\mathrm{C}$ can be found in the work of Cambier and Nauenberg (1986). They calculate the numbers $S(s, K, h)$, giving the average number of sites in the perimeter (the set of nearest-neighbour sites of a cluster) of clusters of s sites when the Ising model is at inverse temperature K and in a magnetic field h. At the $d=2$ Ising critical point they find

$$S(s, K_{\mathrm{c}}, 0)\sim s^{\sigma} \tag{21}$$

with $\sigma=0.68\pm0.04$. On the other hand, the average size R_s of a cluster of s sites (for large s) is determined by the fractal dimensions $\bar{d}$ and is given by

$$R_s\sim s^{1/\bar{d}} \tag{22}$$

giving

$$S(s, K_{\mathrm{c}}, 0)\sim R_s^{\sigma\bar{d}}. \tag{23}$$

The exponent $\sigma\bar{d}$ in (23) can be interpreted as the fractal dimension $\bar{d}_{\mathrm{p}}$ of the perimeter. Using $\sigma=0.68\pm0.04$, and our result $\bar{d}=\frac{187}{96}$, we get $\bar{d}_{\mathrm{p}}=\sigma\bar{d}=1.32\pm0.08$. Of course, the perimeter consists of both the hull and the inner perimeter (the set of sites on the perimeter which are linked to infinity by a path crossing the cluster). Now, if the fractal dimension of the inner perimeter is less than or equal to the hull dimension, which in the case of correlated percolation seems reasonable, the numerical work of Cambier and Nauenberg (1986) leads to

$$\bar{d}_{\mathrm{H}}=\bar{d}_{\mathrm{p}}=1.32\pm0.08 \tag{24}$$

consistent with (20). Taking everything together, these results further confirm the relation between Ising clusters and tricritical $q=1$ Potts model exponents.

To conclude, we made accurate numerical calculations of the fractal dimensions $\bar{d}$ and $\bar{d}_s$ of the incipient infinite Ising cluster. Though some previous estimates of $\bar{d}$ existed we believe that our results are much more accurate. Our result for $\bar{d}_s$ is, to our knowledge, completely new. The results for the exponents y_H and y'_H are consistent with the conjectures $y_H=\frac{187}{96}$, $y'_H=\frac{5}{6}$ and are supporting a recent result according to which critical Ising clusters can be described by tricritical $q = 1$ Potts model exponents. The fractal dimension of the hull $\bar{d}_H$ is then equal to $\frac{11}{8}$, a value consistent with the numerical work of Cambier and Nauenberg (1986).

One of us (CV) would like to thank the IUAP-Belgium for financial support.

References

Balbão D B and Drugowich de Felicio J R 1987 *J. Phys. A: Math. Gen.* **20** L207

Barber M N 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowitz (New York: Academic) p 145

Binder K 1976 *Ann. Phys., NY* **98** 390

Cambier J L and Nauenberg M 1986 *Phys. Rev.* B **34** 8071

Cardy J 1984 *Nucl. Phys.* B **240** 514

—— 1986 *Nucl. Phys.* B **275** 200

—— 1987 *Phase Transitions and Critical Phenomena* vol 11, ed C Domb and J L Lebowitz (New York: Academic) p 55

Coniglio A and Klein W 1980 *J. Phys. A: Math. Gen.* **13** 2775

Coniglio A, Nappi C, Peruggi F and Russo L 1977 *J. Phys. A: Math. Gen.* **10** 205

De'Bell K 1980 *J. Phys. C: Solid State Phys.* **13** 3809

Essam 1980 *Rep. Prog. Phys.* **43** 833

Fisher M E 1967 *Physics (NY)* **3** 255

Friedan D, Qiu Z and Shenker S 1984 *Phys. Rev. Lett.* **52** 1575

Mandelbrot B 1982 *The Fractal Geometry of Nature* (San Francisco: Freeman)

Nienhuis B 1987 *Phase Transitions and Critical Phenomena* vol 11, ed C Domb and J L Lebowitz (New York: Academic) p 1

Nightingale P 1982 *J. Appl. Phys.* **53** 7927

Pietronero L and Tosatti E 1986 *Fractals in Physics* (Amsterdam: North-Holland)

Saleur H and Duplantier B 1987 *Phys. Rev. Lett.* **58** 2325

Stanley H E 1977 *J. Phys. A: Math. Gen.* **10** L211

Stauffer D 1985 *Introduction to Percolation Theory* (London: Taylor and Francis)

Stella A L and Vanderzande C 1988 *Preprint*

Suzuki N 1983 *Prog. Theor. Phys.* **69** 65

Sykes M F and Gaunt D S 1976 *J. Phys. A: Math. Gen.* **9** 2131

Temesvári T and Herényi L 1984 *J. Phys. A: Math. Gen.* **17** 1703

Vanderzande C 1988 *J. Phys. A: Math. Gen.* **21** 833

Vanderzande C and Stella A L 1987 *J. Phys. A: Math. Gen.* **20** 3001

Wu F Y 1982 *Rev. Mod. Phys.* **54** 235