Corrections to scaling in geometrical clusters of the 2D Ising model

View the article online for updates and enhancements.

Corrections to scaling in geometrical clusters of the 2D Ising model

Michail Akritidis[1], Nikolaos G Fytas[1], and Martin Weigel[2] [1]

[1] Centre for Fluid and Complex Systems, Coventry University, Coventry, CV1 5FB, United Kingdom

[2] Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

E-mail: akritidm@uni.coventry.ac.uk

Abstract.
  We study the scaling of the average cluster size and percolation strength of geometrical clusters for the two-dimensional Ising model. By means of Monte Carlo simulations and a finite-size scaling analysis we discuss the appearance of corrections to scaling for different definitions of cluster sets. We find that including all percolating clusters, or excluding only clusters that percolate in one but not the other direction, leads to smaller corrections to scaling for the average cluster size as compared to the other definitions considered. The percolation strength is less sensitive to the definitions used.

1. Introduction

Percolation theory [1] is closely linked to critical phenomena in spin models, as it provides geometrical insights regarding the nature of the transition. The percolation problem is defined through clusters of occupied sites or bonds on a lattice, and one studies the geometrical transition at the percolation threshold, characterized by an incipient spanning cluster that becomes infinite in the thermodynamic limit. The q-state Potts model can be mapped onto a percolation process, by constructing clusters of neighbouring spins with the same orientation. Unfortunately, these *geometrical* clusters do not in general percolate at the critical temperature T_c of the actual phase transition, and they hence do not properly describe the thermal correlations of the system (see [2, 3] for a review). Using a different cluster definition where bonds of neighbouring like spins are deleted with a certain temperature-dependent probability, Fortuin and Kasteleyn (FK) [4] showed that the model can be mapped onto a modified percolation process, where clusters percolate at T_c and, more importantly, they encode the critical behaviour of the system, resulting in the same set of critical exponents. The FK clusters are also the core idea behind the powerful Monte Carlo algorithms of Swendsen and Wang [5] and Wolff [6], where entire FK clusters are flipped instead of individual spins as in the standard Metropolis algorithm [7]. The main advantage of these non-local cluster updates over the local spin flips is the reduction of autocorrelation times in the vicinity of the critical point, significantly improving the simulation efficiency.

  Although geometrical clusters do not capture the critical behaviour, in the two-dimensional (2D) Potts model they at least do percolate at T_c. It turns out that for $0 \leq q \leq 4$ the critical behaviour of geometrical clusters for the pure model is related to the tricritical behaviour of a

diluted Potts model [8, 9]. Stella and Vanderzande [10, 11] showed that the geometrical clusters of the $q = 2$ Potts model, i.e., the Ising model, follow the tricritical behaviour of the $q = 1$ site diluted Potts model. This aspect was numerically verified in references [8, 9].

In the present study we investigate numerically the critical behaviour of the geometrical clusters of the square-lattice Ising model, whose Hamiltonian reads

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j, \tag{1}$$

where the spins take on the values ± 1, $J > 0$ is the ferromagnetic exchange interaction, and the sum extends over all nearest neighbours of the lattice. Specifically, we estimate the exponents of the average cluster size and percolation strength for different sets of clusters, while monitoring the existence of corrections to scaling in each case.

2. Observables

As in random percolation [1], the quantities of interest are the percolation strength P_∞, which gives the fraction of sites belonging to the infinite cluster in the thermodynamic limit, and the average cluster size

$$S = \frac{\sum_{s'} s^2 \, n_s}{\sum_{s'} s \, n_s}, \tag{2}$$

where s denotes the size (number of spins) of the cluster and n_s the number of clusters with size s. The notation s' indicates that the sums are restricted to different sub-sets of clusters, which for the present study are:

(i) All clusters are included: C.
(ii) Exclude the largest cluster in each measurement: $C \setminus \max C$.
(iii) Exclude all percolating clusters: $C \setminus P$.
(iv) Exclude all clusters percolating in horizontal and in vertical direction: $C \setminus P_{\text{x and y}}$.
(v) Exclude all clusters percolating in one specific direction, e.g., horizontal: $C \setminus P_{\text{x}}$.
(vi) Exclude all clusters percolating in one but not the other direction, e.g., horizontal and not vertical: $C \setminus P_{\text{x and } \bar{\text{y}}}$.

For finite size systems P_∞ is usually estimated by the fraction of sites belonging to the largest cluster. Following the idea of cluster sets for S, we can introduce similar sets for P_∞. In the present study we consider, in each configuration, the fraction of sites that belong to the:

(i) Largest cluster: $\max C$.
(ii) Largest percolating cluster: $\max P$.
(iii) Largest cluster that percolates in horizontal and in vertical direction: $\max P_{\text{x and y}}$.
(iv) Largest cluster that percolates in one specific direction, e.g., horizontal: $\max P_{\text{x}}$.
(v) Largest cluster that percolates in one but not the other direction, e.g., horizontal and not vertical: $\max P_{\text{x and } \bar{\text{y}}}$.

In the vicinity of the critical point these observables exhibit a scaling behaviour of the form [1]

$$P_\infty (L, T) = L^{-\beta/\nu} f_{P_\infty} \left[(T - T_{\text{c}}) L^{1/\nu} \right], \tag{3}$$

$$S (L, T) = L^{\gamma/\nu} f_S \left[(T - T_{\text{c}}) L^{1/\nu} \right], \tag{4}$$

where ν is the critical exponent of the correlation length, γ the critical exponent that captures the divergence of the average cluster size, and β the critical exponent which describes how the strength of the percolating cluster goes to zero as T_{c} is approached from below. f_{P_∞} and f_S are universal finite-size scaling functions.

3. Results

We simulated the 2D Ising model with periodic boundary conditions using the Swendsen-Wang algorithm [5]. We considered systems of linear size $L = 16, 32, 64, 128, 256, 512, 600, 1000, 1200, 1600$ and 2000, at the exact critical temperature $T_c = 2/\ln\left(1 + \sqrt{2}\right)$. For all L the total number of simulation steps was $1.1 \times \tau_{\text{int, E}} \times 10^5$ sweeps, where $\tau_{\text{int, E}}$ is the integrated autocorrelation time of the energy [12], and $\tau_{\text{int, E}} \times 10^4$ sweeps were discarded during equilibration. After every $\tau_{\text{int, E}}$ sweeps a measurement was taken, leading to up to 10^5 measurements per run. The estimates of $\tau_{\text{int, E}}$, rounded up to the next largest integer, in ascending order of the system size are: $\tau_{\text{int, E}} = 4, 5, 5, 6, 7, 9, 9, 10, 11, 11, 12$ sweeps. Statistical errors were estimated by means of jackknife blocking [13]. We considered a cluster to percolate in one direction if it wraps around this direction and is connected back to itself. To identify the wrapping clusters, we employed the method of Machta *et al.* [14].

At T_c, according to equations (3) and (4), $f_P(0) = \text{const.}$ and $f_S(0) = \text{const.}$, allowing the estimation of γ/ν and β/ν as a function of L. For all sets of clusters, fits were performed using the least-squares Levenberg-Marquardt algorithm [15]. In order to obtain the influence of corrections to scaling in the observables we performed fits including $L_{\min} \leq L \leq L_{\max}$, by systematically increasing the lower cut-off $L_{\min}$, while the upper cut-off is kept fixed $L_{\max} = 2000$.

In figure 1(a) the average cluster size as a function of L is plotted for the different definitions introduced in section 2. Visually, the data of all definitions seem to follow straight lines, on a log-log plot, indicating merely small corrections to scaling. Estimates of γ/ν for different fit intervals and the respective quality-of-fit parameter Q are reported in table 1. For C and $C \setminus P_{\text{x and } \overline{y}}$, γ/ν converges relatively quickly to its asymptotic value, $\gamma/\nu = 91/48 \approx 1.896$ [10] as $L_{\min}$ increases. Specifically, the discrepancy from the asymptotic value is less than 3 standard deviations (3σ) for $L_{\min} \geq 64$ and $L_{\min} \geq 256$ respectively, so that corrections to scaling are not substantial. This is nicely illustrated in figure 1(b), where the exponent γ/ν is plotted as a function of $1/L_{\min}$. For $C \setminus P_{\text{x and y}}$, $C \setminus P_{\text{x}}$, $C \setminus \max C$, and $C \setminus P$, on the other hand, the convergence to the asymptotic value is found to be very slow. Even for $L_{\min} = 1200$, the deviation from the asymptotic values is around 6σ for all definitions, indicating that corrections to scaling are important. This is illustrated in figure 1(b), where the estimates of the exponent seem to converge to a value significantly below the predicted one. The fact that C and $C \setminus P_{\text{x and } \overline{y}}$ give similar results is to be expected. Percolating clusters in one but not the other direction are very rare, thus excluding them from the sums of equation (2) will not affect the average cluster size significantly. This can also be seen from figure 1(a), where the data points for the two definitions, at the same L, are equal within error bars. Note that previous estimates of the exponent using the C definition are reported in reference [16] and these for the $C \setminus P_{\text{x}}$ definition in reference [17].

For the percolation strength, data for all sets seem to follow a straight line on a log-log plot as a function of L, indicating small corrections to scaling, as is shown in figure 2(a). This observation is supported by table 2, where the estimates of β/ν and Q are reported. Setting aside $\max P_{\text{x and } \overline{y}}$, for all sets the deviations from the asymptotic value $\beta/\nu = 5/96 \approx 0.052$ [10] is less than 3σ for all $L_{\min} \geq 64$, indicating rather small corrections to scaling. Notably, for $\max P_{\text{x and y}}$ deviations are even smaller than 1.7σ for all $L_{\min}$. According to table 2 the estimates of β/ν for $\max P_{\text{x and } \overline{y}}$ are less than 3σ from the asymptotic value (except $L_{\min} = 16$), but the statistical errors are large, thus not allowing a reasonable estimate of the exponent. The explanation for this behaviour of $\max P_{\text{x and } \overline{y}}$ is in line with the $C \setminus P_{\text{x and } \overline{y}}$ for the average cluster size, but going in the opposite direction. As already stated above, clusters percolating in one but not the other direction are rare, leading to poor statistics and larger statistical errors for the percolation strength; see figure 2(b), where the exponent β/ν is plotted as a function of $1/L_{\min}$.
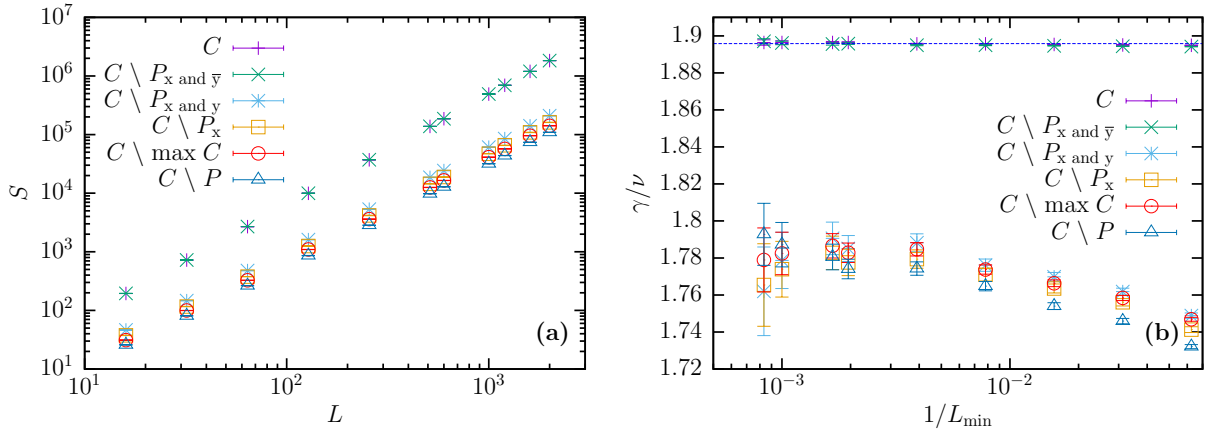
Figure 1. (a) Log-log plot of the average cluster size as a function of L for the different definitions. (b) Exponent ratio γ/ν as a function of $1/L_{\min}$. The dashed horizontal line marks the asymptotic value $91/48 \approx 1.896$ [10].

Table 1. Estimates of γ/ν, quality-of-fit parameter Q, and deviations from the exact value, $\gamma/\nu = 91/48 \approx 1.896$, in multiples of the estimated statistical errors $\Delta(\sigma)$, for the cluster sets of the average cluster size as introduced in section 2.

	C			$C \setminus P_{\text{x and } \overline{\text{y}}}$			$C \setminus P_{\text{x and y}}$		
$L_{\min}$	γ/ν	Q	$\Delta(\sigma)$	γ/ν	Q	$\Delta(\sigma)$	γ/ν	Q	$\Delta(\sigma)$
16	1.89490(11)	0.001	8.28	1.89419(11)	0.001	15.03	1.7488(14)	0.000	101.59
32	1.89510(14)	0.010	5.36	1.89440(13)	0.008	10.76	1.7618(19)	0.000	71.51
64	1.89535(17)	0.044	2.83	1.89465(17)	0.042	7.11	1.770(2)	0.002	53.39
128	1.8957(2)	0.123	0.75	1.8950(2)	0.130	3.94	1.776(3)	0.021	36.14
256	1.8957(3)	0.078	0.52	1.8950(3)	0.079	2.78	1.788(5)	0.658	22.21
512	1.8964(4)	0.723	1.30	1.8958(4)	0.747	0.10	1.785(7)	0.575	15.78
600	1.8964(6)	0.613	1.03	1.8956(6)	0.668	0.46	1.791(9)	0.611	11.97
1000	1.8964(10)	0.568	0.60	1.8962(9)	0.623	0.35	1.779(15)	0.639	7.71
1200	1.8964(14)	0.300	0.40	1.8971(14)	0.628	0.86	1.76(2)	0.778	5.59

|	$C \setminus P_{\text{x}}$			$C \setminus \max C$			$C \setminus P$		
$L_{\min}$	γ/ν	Q	$\Delta(\sigma)$	γ/ν	Q	$\Delta(\sigma)$	γ/ν	Q	$\Delta(\sigma)$
16	1.7413(16)	0.000	99.00	1.7469(11)	0.000	140.19	1.7321(11)	0.000	148.24
32	1.756(2)	0.000	70.11	1.7584(14)	0.000	97.21	1.7459(15)	0.000	102.89
64	1.764(2)	0.016	54.90	1.7663(18)	0.000	70.59	1.7540(18)	0.000	76.73
128	1.771(3)	0.307	37.30	1.774(2)	0.003	48.41	1.765(3)	0.008	52.35
256	1.779(5)	0.875	23.45	1.785(4)	0.868	30.87	1.774(4)	0.514	33.64
512	1.778(7)	0.794	16.59	1.783(5)	0.806	21.64	1.774(5)	0.374	23.01
600	1.783(9)	0.847	12.52	1.787(7)	0.860	16.57	1.781(7)	0.544	16.65
1000	1.774(15)	0.873	8.11	1.782(11)	0.754	9.87	1.787(12)	0.431	9.04
1200	1.77(2)	0.969	5.85	1.779(17)	0.484	6.76	1.793(17)	0.228	6.15
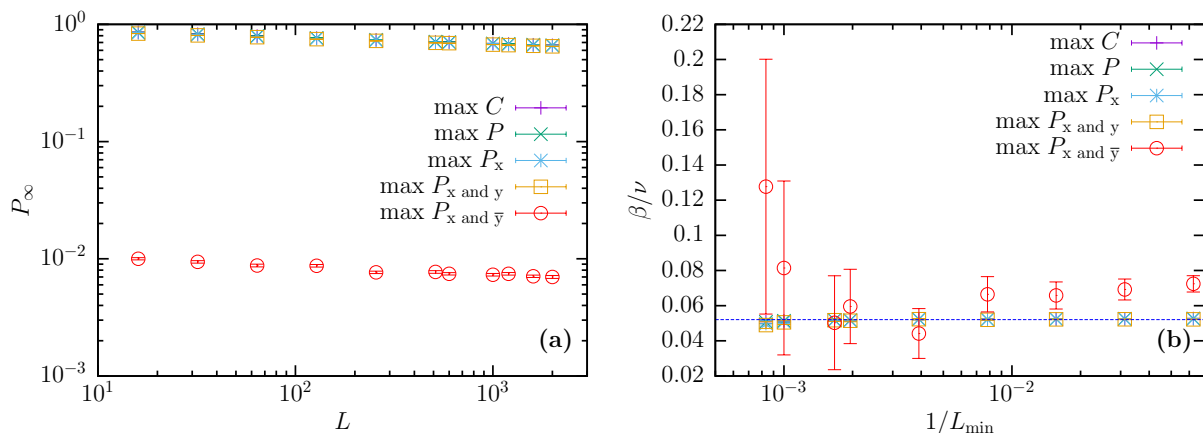
Figure 2. (a) Log-log plot of the strength as a function of L for the different definitions. (b) Exponent ratio β/ν as a function of $1/L_{\min}$. The dashed horizontal line marks the asymptotic value $5/96 \approx 0.052$ [10].

Table 2. Estimates of β/ν, quality-of-fit parameter Q, and deviations from the exact value, $\beta/\nu = 5/96 \approx 0.052$, in multiples of the estimated statistical errors $\Delta\,(\sigma)$, for the cluster sets of the percolation strength as introduced in section 2.

	max C			max P			max P_{x}		
$L_{\min}$	β/ν	Q	$\Delta\,(\sigma)$	β/ν	Q	$\Delta\,(\sigma)$	β/ν	Q	$\Delta\,(\sigma)$
16	0.05271(8)	0.005	7.94	0.05269(8)	0.008	7.65	0.05245(11)	0.230	3.30
32	0.05256(10)	0.030	4.94	0.05255(10)	0.036	4.76	0.05243(14)	0.166	2.56
64	0.05241(12)	0.081	2.66	0.05240(12)	0.092	2.55	0.05236(16)	0.136	1.68
128	0.05222(17)	0.141	0.81	0.05222(17)	0.136	0.83	0.0521(2)	0.216	0.06
256	0.0523(2)	0.109	1.14	0.0523(2)	0.103	1.13	0.0522(3)	0.156	0.43
512	0.0517(3)	0.744	1.06	0.0517(3)	0.718	1.07	0.0515(5)	0.597	1.32
600	0.0519(4)	0.670	0.44	0.0519(4)	0.653	0.42	0.0517(6)	0.494	0.70
1000	0.0514(7)	0.671	0.96	0.0514(7)	0.678	0.99	0.0507(9)	0.681	1.45
1200	0.0509(11)	0.586	1.17	0.0508(11)	0.600	1.19	0.0498(14)	0.955	1.61

	max $P_{\text{x and y}}$			max $P_{\text{x and }\overline{\text{y}}}$			-	-	-
$L_{\min}$	β/ν	Q	$\Delta\,(\sigma)$	β/ν	Q	$\Delta\,(\sigma)$			
16	0.05224(14)	0.232	1.17	0.072(5)	0.432	4.38			
32	0.05227(17)	0.169	1.08	0.069(6)	0.402	2.87			
64	0.0522(2)	0.119	0.66	0.066(8)	0.347	1.78			
128	0.0520(3)	0.135	0.42	0.066(10)	0.251	1.43			
256	0.0523(4)	0.153	0.60	0.044(14)	0.730	0.56			
512	0.0514(6)	0.508	1.14	0.06(2)	0.763	0.35			
600	0.0517(7)	0.435	0.48	0.05(3)	0.676	0.07			
1000	0.0505(12)	0.569	1.30	0.08(5)	0.617	0.59			
1200	0.0490(19)	0.881	1.64	0.13(7)	0.651	1.04			

5

4. Summary

Using several classes of sub-sets of clusters we determined the critical exponents for the average cluster size and percolation strength for geometrical clusters in the 2D Ising model. Our data were generated by means of Monte Carlo simulations for systems of linear size up to $L = 2000$. Estimates of the exponents for all cluster sets using finite-size scaling were reported, while the appearance of corrections to scaling was monitored by performing fits on intervals $L_{\min} \leq L \leq L_{\max}$ with increasing $L_{\min}$. Overall, where corrections to scaling are not very strong, our results are in agreement with exact values within error bars and the numerical accuracy allowed us to draw conclusions for the presence of scaling corrections.

The average cluster size is sensitive to the exclusion of certain classes of clusters. Excluding percolating clusters (except clusters percolating in one but not the other direction) or the largest cluster, which is commonly done in numerical studies of random percolation [1], leads to strong corrections to scaling. On the other hand, when all clusters are included, minimal corrections to scaling appear. This is also valid when percolating clusters in one but not the other direction are excluded, but mainly because these clusters appear less often.

The percolation strength is less sensitive to the definitions used. Except from the case of $\max P_{\mathrm{x \ and \ \overline{y}}}$, the rest provide reasonable estimates of the involved exponent with rather small corrections. The low probability of clusters that percolate in one but not the other direction, leads to poor statistics resulting in estimates of very low accuracy compared to the other definitions been used.

As the average cluster size of the full set C does not show any maximum as a function of temperature, estimates of pseudo-critical temperatures need to be extracted from other quantities in cases where the transition temperature is not known exactly. A more systematic analysis, allowing one to quantify the corrections to scaling would be an interesting task for future work. The inclusion of additional sets of clusters is also feasible, and could presumably lead to optimal sets of definitions for the observables under consideration, with minimal corrections to scaling, thus allowing accurate estimates of the critical exponents.

Acknowledgments

References

[1] Stauffer D and Aharony A 1994 *Introduction to percolation theory* 2nd ed (London: Taylor & Francis)
[2] Coniglio A and Fierro A 2009 *Encyclopedia of Complexity and Systems Science* ed Meyers R A (New York: Springer) p 1596
[3] Saberi A A 2015 *Phys. Rep.* **578** 1
[4] Fortuin C M and Kasteleyn P W 1972 *Physica* **57** 536
[5] Swendsen R H and Wang J S 1987 *Phys. Rev. Lett.* **58** 86
[6] Wolff U 1989 *Phys. Rev. Lett.* **62** 361
[7] Metropolis N, Rosenbluth A W, Rosenbluth M N, Teller A H and Teller E 1953 *J. Chem. Phys.* **21** 1087
[8] Janke W and Schakel A M J 2004 *Nucl. Phys. B* **700** 385
[9] Janke W and Weigel M 2006 *Phys. Lett. B* **639** 373
[10] Stella A L and Vanderzande C 1989 *Phys. Rev. Lett.* **62** 1067
[11] Vanderzande C and Stella A L 1989 *J. Phys. A* **22** L445
[12] Weigel M and Janke W 2010 *Phys. Rev. E* **81** 066701
[13] Efron B and Tibshirani R J 1993 *An Introduction to the Bootstrap* (New York: Chapman and Hall/CRC)
[14] Machta J, Choi Y S, Lucke A, Schweizer T and Chayes L M 1996 *Phys. Rev. E* **54** 1332
[15] Press W H, Teukolsky S A, Vetterling W T and Flannery B P 1996 *Numerical Recipes in FORTRAN 77: The Art of Scientific Computing* vol 1 (Cambridge: Cambridge University Press) p 678 2nd ed
[16] Janke W and Schakel A M J 2005 *Phys. Rev. E* **71** 036703
[17] Fortunato S 2002 *Phys. Rev. B* **66** 054107