

## Critical phenomena on $k$ -booklets

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We define a “ $k$ -booklet” to be a set of  $k$  semi-infinite planes with  $-\infty < x < \infty$  and  $y \geq 0$ , glued together at the edges (the “spine”)  $y = 0$ . On such booklets we study three critical phenomena: self-avoiding random walks, the Ising model, and percolation. For  $k = 2$ , a booklet is equivalent to a single infinite lattice, and for  $k = 1$  to a semi-infinite lattice. In both these cases the systems show standard critical phenomena. This is not so for  $k \geq 3$ . Self-avoiding walks starting at  $y = 0$  show a first-order transition at a shifted critical point, with no power-behaved scaling laws. The Ising model and percolation show hybrid transitions, i.e., the scaling laws of the standard models coexist with discontinuities of the order parameter at  $y \approx 0$ , and the critical points are not shifted. In the case of the Ising model, ergodicity is already broken at  $T = T_c$ , and not only for  $T < T_c$  as in the standard geometry. In all three models, correlations (as measured by walk and cluster shapes) are highly anisotropic for small  $y$ .

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Critical phenomena are usually considered either on regular lattices or on random graphs. What happens if these are replaced by geometries that are regular lattices *nearly* everywhere, but are atypical at subdomains of measure zero?

The best known cases are semi-infinite lattices with  $d$  bulk dimensions and with one  $(d - 1)$ -dimensional surface. The Ising model on a simple cubic lattice restricted to  $z = 0$  is maybe the most studied model of that type. If the surface bonds are not much stronger than the bulk bonds (“ordinary transition”), the magnetization slightly below  $T_c$  is weaker at the surface than in the bulk and the surface order parameter exponent is larger than the bulk exponent,  $\beta_1 > \beta$ . At the other extreme of very strong surface bonds (“extraordinary transition”), the surface can already order when the bulk is still disordered and the scaling at  $T_c$  is that of the “normal” transition with an applied nonzero magnetic field at the surface [1].

The situation is very similar for other critical phenomena, such as percolation or self-avoiding walks (SAWs). In all these cases there is a special point where the strength of the surface bonds (or contacts in the case of SAWs) is just sufficient to compensate the disordering effect of the absent bonds with  $z < 0$ . If the surface bounds or contacts, respectively, are stronger than the special value, the surface orders already when the bulk is still disordered.

This scenario has to be modified for  $d = 2$ , where the surface has  $d = 1$ . In that case neither the Ising model nor percolation can order at the surface at any finite control parameter. Thus extraordinary and special transitions do not exist for them, while they do exist for SAWs [2].

But this is not yet the end of the story. Consider  $k$  semi-infinite planes with  $y \geq 0$ , glued together at the edges  $y = 0$ . If  $k > 2$ , we can expect that random fluctuations of the order parameter at  $y = 0$  can reinforce each other. If going from  $k = 2$  (infinite plane) to  $k = 1$  (semi-infinite plane) tends to disorder the lattice, we can envisage that going to  $k > 2$  will lead to increased ordering. This is indeed true, but the details are nontrivial.

For simplicity, in the following we shall consider only square lattices. Locally, the only difference between lattice sites on and off the spine is just their coordination number.

While it is 4 for all sites off the spine, it is  $2 + k$  on the spine. Apart from this, the spine is treated in the algorithms used in this Rapid Communication (which are all growth algorithms) as the rest of the system.

Recently, I became aware that the Ising model on  $k$ -booklets (called there “multiple junctions”) had been studied before by means of renormalization group methods [3,4]. Also recently, directed percolation was studied on multiple junctions [5]. Although the methods used in Refs. [3,4] were very different, as are also the details observed in Ref. [5], these papers fully support our results.

*Self-avoiding walks.* For SAWs on the infinite square lattice, the number of walks of length  $N$  scales as

$$Z_N \sim N^{\gamma-1} \mu^N, \quad (1)$$

where the *connective constant* is  $\mu = 2.638\,158\,53\dots$  [6], and the entropic exponent is  $\gamma = 43/32$  [7]. Therefore, when plotting  $Z_N/\mu^N$  against  $N$ , we expect a power law with exponent  $\gamma - 1 \approx 0.344$ . Analogously, we assume that the number of SAWs starting at  $y = 0$  for any  $k$  increases with connective constant  $\mu_k$ , up to possible powers of  $N$ . In Fig. 1 we show  $\ln Z_N - \mu_k^N$ , obtained with the pruned-enriched Rosenbluth method (PERM) algorithm [8], for  $N$  up to  $N = 10\,000$  and for  $k = 1, 2, 3, 4$ , and 6. For  $k = 1$  and  $k = 2$ , we have  $\mu_k = \mu$ , and  $\gamma$  is nontrivial. On the other hand, for  $k > 2$ , the fitted values of  $\mu_k$  increase with  $k$ , while  $\gamma = 1$ .

These simulations also show that the spatial extents of walks in the  $x$  and  $y$  directions scale with the Flory exponent for  $k = 1$  and  $k = 2$ , while they are very different for  $k > 2$ . More precisely, the longitudinal rms end-to-end distance  $\sqrt{\langle x^2 \rangle}$  increases for large  $N$  linearly with  $N$ , while  $\sqrt{\langle y^2 \rangle}$  stays finite and reaches a constant (see Fig. 2). Indeed, we find also that distributions of  $y$  do not follow power laws for  $k > 2$  (as they do for  $k = 1$  and 2), but are exponentials (data not shown). All this means that self-avoiding walks are strongly attracted to the spine for  $k \geq 3$ , to the extent that the transverse correlation length is finite, and the growth is ballistic in the direction of the spine. Thus all aspects of criticality of the model on single planes are gone.

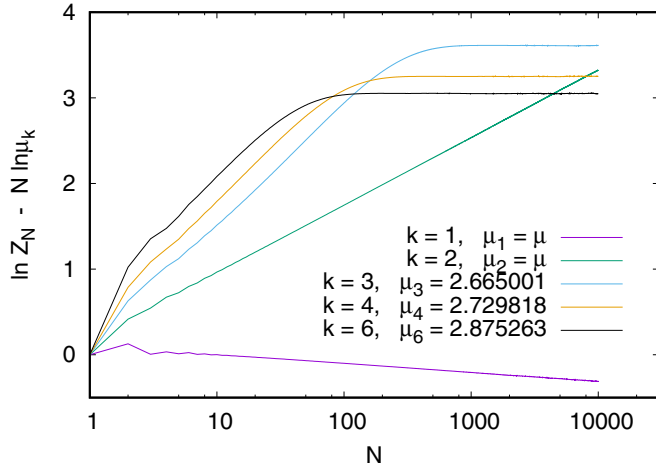


FIG. 1. Log-log plot of average numbers of self-avoiding walks of length  $N$  on  $k$  joined semi-infinite planes, divided by  $\mu_k^N$ . Here,  $\mu_1 = \mu_2 = \mu$  is the known connective constant of SAWs on ordinary square lattices, while  $\mu_k$  for  $k > 2$  are connective constants fitted from these data. For  $k \leq 2$ , the  $\gamma$  exponents are in agreement with  $\gamma_1 = 61/64$  [9] and  $\gamma_2 = \gamma = 43/32$  [7], while they are equal to 1 for  $k > 2$ .

*Ising model.* We simulated the Ising model with the Wolff algorithm [10]. Boundary conditions were periodic at the sides  $x = 0$  and  $x = L$ , but open at  $y = L$ . We only show data for the bulk critical temperature, as we saw no hint that the critical point is shifted as it happened for SAWs. The main observables were the average squared magnetization at fixed  $y$  and the finite size scaling of its distribution at  $y = 0$ . Plots of  $\langle m^2(y) \rangle$  for  $L = 1000$  are shown in Fig. 3. All curves fall off for large  $L$  because of the open boundary conditions at  $y = L$ . For small  $y$ , we see that the curve is flat for  $k = 2$ , as we expect. It scales for  $k \geq 3$  as

$$\langle m^2(y) \rangle \sim y^{-2\beta/\nu}, \quad (2)$$

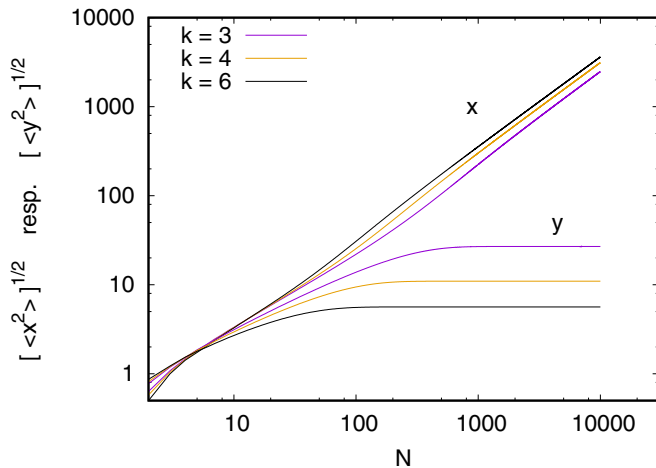


FIG. 2. Log-log plot of rms end-to-end distances of self-avoiding walks in the directions parallel and perpendicular to the spine, for  $k = 3, 4$ , and  $6$ . We do not show the data for  $k = 1$  and  $2$ , since they scale according to the well-known Flory exponent,  $[\langle x^2 \rangle]^{1/2} \sim [(\langle y^2 \rangle)]^{1/2} \sim N^{3/4}$ . The asymptotic scaling is reached fastest for  $k = 6$ , and slowest for  $k = 3$ .

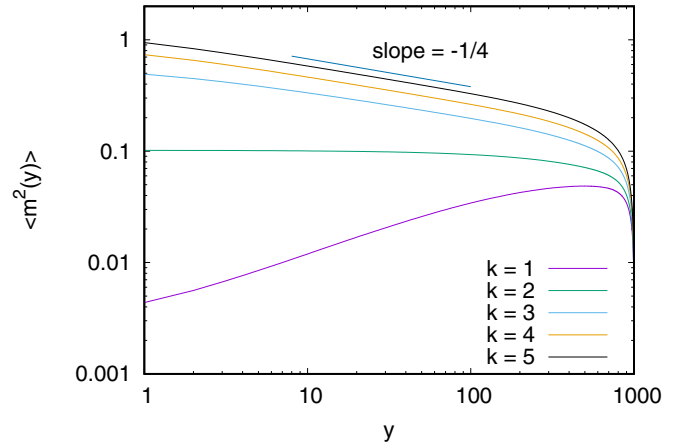


FIG. 3. Log-log plot of the average squared magnetization density at fixed  $y$ , for  $k$  Ising models joined at  $y = 0$ . The temperature is the critical one for single lattices.

with  $\beta/\nu = 1/8$ , as expected for a normal surface with nonzero applied surface field. This indicates that the mutual reinforcement of the  $k$  sheets is sufficient to order the system at the spine.

The same is also indicated by the distributions of the magnetization at  $y = 0$ . In Fig. 4 we show results for  $k = 2$

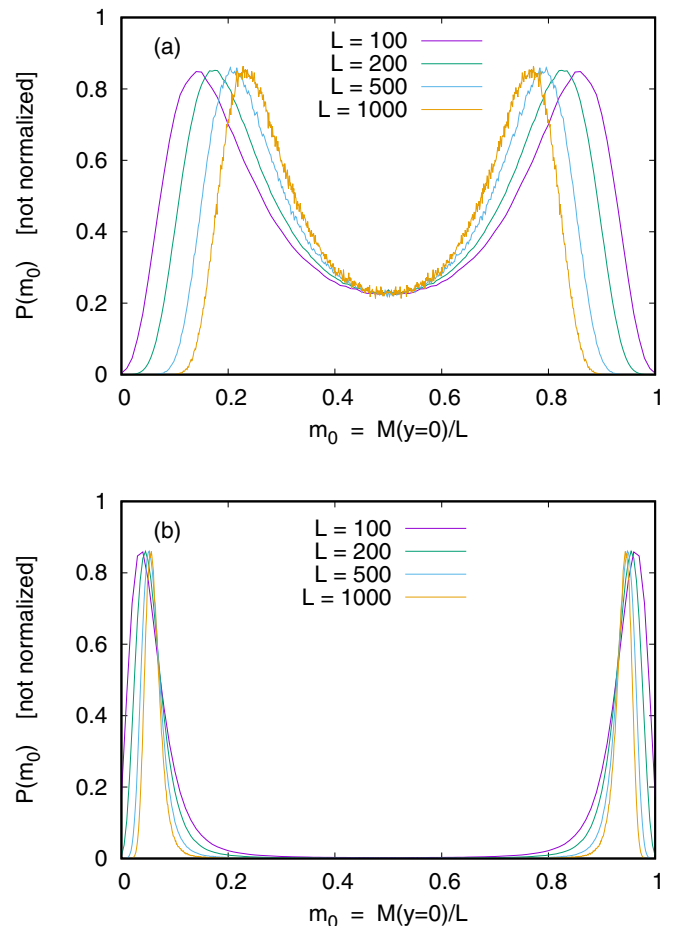


FIG. 4. Non-normalized distributions of the Ising magnetization densities at  $y = 0$ , (a) for  $k = 2$  and (b) for  $k = 3$ .

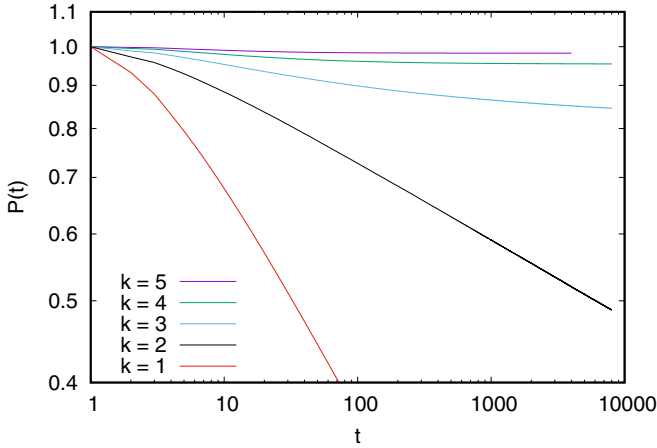


FIG. 5. Probabilities  $P(t)$  that a percolation cluster at  $p = p_c$  continues to grow for time  $\geq t$ . Clusters start growing at the line  $y = 0$ .

(top panel) and  $k = 3$  (bottom panel). All distributions are not normalized. For  $k = 2$ , we see the usual finite size scaling for second-order phase transitions [11]

$$P(m) \propto \Phi(mL^{\beta/\nu}), \quad (3)$$

i.e., the curves are just rescaled when  $L$  is changed. This is not the case for  $k = 3$ , where the two peaks become sharper as  $L$  increased, and the valley between them becomes deeper. This is the hallmark of a first-order phase transition. Moreover, due to the increasing depth of the valley, magnetization switches become rarer with increasing  $L$ . Thus ergodicity is for large systems already broken at  $T = T_c$ , and not only for  $T < T_c$  as for single-sheeted lattices. Notice, however, that at the same time we have power-behaved correlations at large  $y$ , i.e., we have a hybrid case where the discontinuous jump of the order parameter at  $y = 0$  coexists with a continuous transition for  $y \gg 0$ .

*Percolation.* Finally, we shall discuss the case of percolation. More precisely, we study site percolation by means of the Leith algorithm, which allows us to start cluster growth from a single site at a specific value of  $y$ . We concentrate of course on clusters grown from  $y = 0$ . We use the breadth-first version of the Leith algorithm, and denote by  $t$  the “time,” i.e., the number of spreading steps needed to reach a site.

In a first set of runs we used  $p = p_c = 0.592\,746\,05$  [12], stopped the growth at  $t = t_{\max}$ , and used lattices that were large enough so that the boundaries were never reached. In Fig. 5 we show the probabilities  $P(t)$  that a cluster starting at  $y = 0$  continues to grow at least for  $t$  time steps. For  $k = 1$  and  $k = 2$ , it is known that  $P(t)$  obeys a power law  $P_k(t) \sim t^{-\delta_k}$ , with  $\delta_k = \beta_k/\nu/d_{\min}$ , where  $\nu = 4/3$  [13],  $d_{\min} = 1.130\,77(2)$  [14],  $\beta_1 = 4/9$ , and  $\beta_2 = \beta = 5/36$  [15]. For  $k \geq 3$ , it seems that  $P(t)$  converges towards a positive value for  $t \rightarrow \infty$ . Assuming an ansatz  $P(t) = P(\infty) - a/t^\Delta$ , we obtained  $P(\infty) = 0.813(5)$  and  $\Delta = 0.22(2)$  for  $k = 3$ , while we got  $P(\infty) = 0.954(4)$  and  $\Delta = 0.6(1)$  for  $k = 4$ .

Notice that this positivity of  $P(\infty)$  is not, in contrast to the case of SAWs, due to the fact that the critical point has shifted for  $k > 2$ , as we shall see explicitly below. Since  $P(\infty)$  is also the probability that a randomly chosen site is

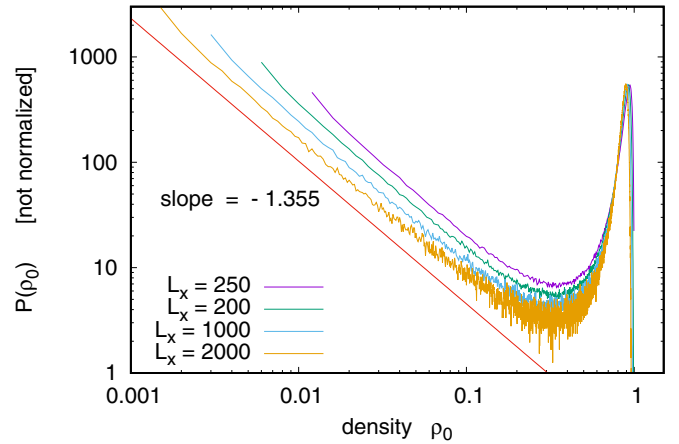


FIG. 6. Non-normalized distributions of the density  $\rho_0$  of sites on the axis  $y = 0$  “wetted” by clusters that start to grow at  $y = 0$ . In these simulations  $L_x$  was finite, but  $L_y$  was so large as to be effectively infinite. The left-hand peak corresponds to clusters that died early, while the right-hand peak corresponds to clusters that grow to values  $y \gg L_x$ .

located on the infinite cluster and is considered as the order parameter, we thus conclude that the order parameter is finite at the critical point for  $k \geq 3$  and for  $y = 0$ , i.e., the model shows some aspect of a first-order transition. To further support this, we made a second set of runs—also at  $p = p_c$ —on lattices of size  $L_x \times L_y$  with  $L_y \gg t_{\max}^{1/d_{\min}} \gg L_x$  and with periodic boundary conditions in the  $x$  direction. Also, here we started the growth at  $y = 0$ . But now times were so large that the clusters that survived for long times covered the  $x$  axis  $\{0 < x < L_x, y = 0\}$  uniformly. If the above scenario with  $P(\infty) > 0$  is correct, we expect then for each run essentially two possibilities: Either the cluster dies soon and the density  $\rho_0$  of “wetted” (or “infected”) sites on the  $x$  axis is small [ $O(1/L_x)$ ], or this density is finite and turns for  $L_x \rightarrow \infty$  towards  $P(\infty)$ .

Data obtained for  $k = 3$  are shown in Fig. 6 and confirm this perfectly: While there are two broad peaks of the density distribution  $P(\rho_0)$  for finite  $L_x$ , they tend towards delta peaks for  $L_x \rightarrow \infty$ . We show non-normalized distributions where the right-hand peaks have the same heights, because then it is most easy to verify that the peak positions do not move with  $L$ , i.e., the density is finite and not fractal. At the left-hand peak we see a scaling law  $P(\rho_0) \sim \rho_0^{-\sigma}$  with  $\sigma = 1.355(10)$ , indicating that there is a new nontrivial exponent for small clusters starting to grow at  $y = 0$ .

Clusters grown at  $y = 0$  for  $k \geq 3$  are strongly anisotropic, as seen also by the growth of  $X_k(t)^2 = \langle x^2 \rangle$  and  $Y_k(t)^2 = \langle y^2 \rangle$ . Here, the seed is assumed to be at  $x = y = 0$ , and the averages are over all active sites at time  $t$ . Data for  $t^{-2}X_k(t)^2$  obtained during the first set of runs are shown in Fig. 7. We do not show the data for  $Y_k(t)^2$  since they are trivial: For all  $k$ , we have  $Y_k(t)^2 \sim t^{2/d_{\min}}$ . This is not so for  $X_k(t)^2$  with  $k > 2$ . Figure 7 strongly suggests nontrivial power laws  $X_k(t)^2 \sim t^{z_k}$  for  $k = 3$  and  $k = 4$  [with  $z_3 = 1.821(1)$  and  $z_4 = 1.91(1)$ ]. But for  $k \geq 5$  we are no longer able to distinguish between such nontrivial scaling laws and trivial power laws  $X_k(t)^2 \sim t^2$  with very long transients.

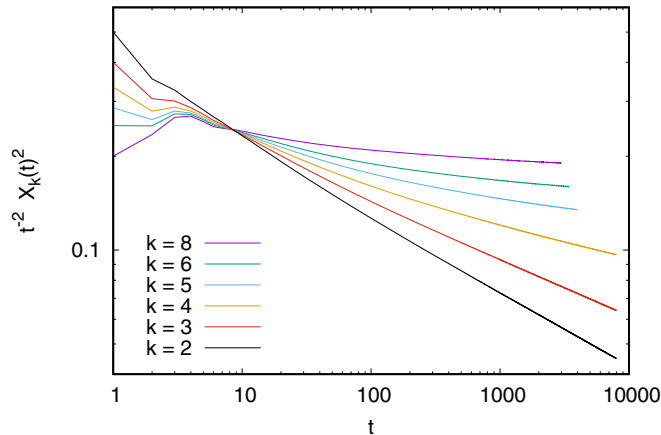


FIG. 7. Log-log plots of the (squared) cluster growth in the  $x$  direction, for  $k = 2, 3, \dots, 8$ . For  $k = 2$ , we have of course the usual growth of two-dimensional (2D) percolation clusters, but for  $k > 2$ , the growth follows power laws with larger exponents.

Finally, in a last set of runs, we estimated the average cluster sizes  $s$  for subcritical values of  $p$ . This time both  $L_x$  and  $L_y$  were large enough so that all clusters died before boundaries were reached. All clusters started to grow at  $y = 0$ . In ordinary percolation [16] we have  $s \sim (p_c - p)^{-\gamma}$ , where  $\gamma = 43/18$  for the bulk and  $\gamma = \gamma_1 = 25/12$  for clusters growing at a boundary [15]. From Fig. 8 we see that this generalizes to arbitrary  $k \geq 1$ , with nontrivial exponents  $\gamma_k$  at least for  $k \leq 5$ . For large  $k$ , we see, however, large corrections to scaling, due to which we cannot give reliable estimates for  $\gamma_k$  with  $k \geq 5$ . In any case, these simulations show clearly that the critical point is not shifted for  $k > 2$ .

*Discussion.* One reason for this study was the aim of finding and studying different cases of hybrid phase transitions. These are transitions that show features of second-order transitions such as anomalous scaling laws, but where also order parameters jump discontinuously as in first-order transitions. During recent years many such cases were found [17–29], but they are still not well understood. In two of our three models (Ising, percolation) the transition is indeed hybrid, while it is not for SAWs. The fact that the transition is hybrid in the Ising case and for directed percolation has also been found in Refs. [3–5].

More fundamentally, it is of interest to study what happens to phase transitions when the underlying structure is a regular lattice *nearly* everywhere—but not everywhere—and has nontrivial global topology. The main examples for this are regular lattices with boundaries. To my knowledge, polymer networks [30] are the only well-studied model where systems with complex topologies are formed by gluing together simple

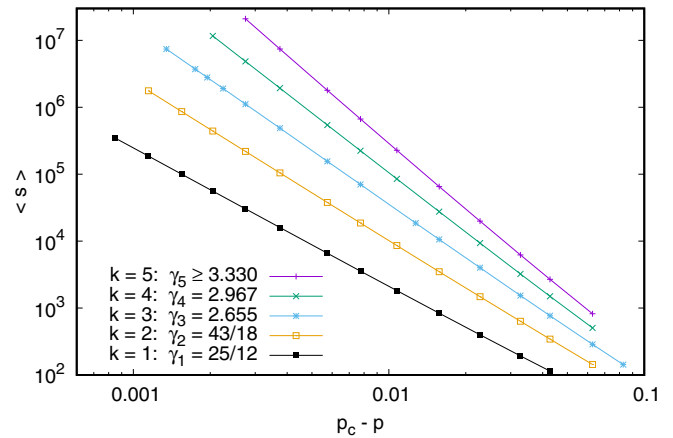


FIG. 8. Log-log plots of average cluster sizes, for subcritical clusters grown from seeds at  $y = 0$  on infinitely large lattices. For  $k \leq 2$ , we recover the known scaling laws, and for  $k \geq 3$ , we find again scaling laws with new exponents.

systems. There, the situation is similar to the percolation case studied here, in the sense that some critical exponents depend on the topology while others do not. We should point out that lattice defects alone—even extended ones as in Ref. [31], where one line in a 2D lattice is different from the rest—do not give rise in the Ising model and in percolation to phenomena similar to the ones discussed here.

Finally, let us discuss possible experimental realizations. The prime example of a 3-booklet is of course three soap films meeting at  $120^\circ$ . Self-avoiding walks can be studied in this geometry by placing a long polymer (e.g., DNA) close to the line where they meet. Due to the changed connective constant, the polymer will be drawn towards it. When it is there, it will be very much stretched to stay as close to the line as possible. The problem is of course more complicated than our toy model, because the soap films are elastic and will deform in response to the polymer [32]. Thus a detailed quantitative analysis would be not easy. Nevertheless, the basic predictions of our model should apply, and it would be an interesting question how much they are modified by film elasticity.

Instead of soap films, one could of course also consider lipid bilayers or other biomembranes, although it might not be so easy to make clean 3-booklets. The advantage over soap films would then be that biomembranes show various phase transitions [33–36]. Studying these transitions on a booklet geometry could then open a wide range of different phenomena.

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