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LETTER TO THE EDITOR

Thermally driven phase transitions near the percolation threshold in two dimensions†

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Abstract. It is shown that thermally driven magnetic critical phenomena just above and just below the percolation limit can be usefully analysed using scaling theory; a further assumption concerning cluster connectivity provides quantitative predictions for critical exponents and scaling functions that should be experimentally testable. In particular, reasonable agreement is found with recent experimental results of Birgeneau, Cowley, Shirane and Guggenheim on the quasi-two-dimensional random magnet $Rb_2Mn_pMg_{1-p}F_4$.

The hypotheses of scaling and universality have provided a useful framework within which to describe thermally-driven phase transitions occurring in a wide variety of physical systems. It is therefore of some interest to study situations in which these hypotheses may be expected to change form or cease to be valid. The percolation limit is one such situation (figure 1(*a*)). Here we consider the 'quenched site percolation problem' (for terminology, see Shante and Kirkpatrick (1971)) in which a fraction p of the sites in a lattice are randomly occupied by magnetic moments. For $p = 1$, the scaling and universality hypotheses are valid (figure 1(*b*)); for $p \lesssim 1$, there is evidence that the scaling hypothesis continues to be valid, at least sufficiently close to the 'critical line' $T_c(p)$‖ (Stoll and Schneider 1976). However, for $p \lesssim p_c$—where p_c denotes the percolation threshold—no phase transition can exist since the system breaks up into isolated finite clusters that cannot sustain long-range order. Thus, at p_c the scaling and universality hypotheses will almost certainly need modification.

The change in 'connectivity of occupied lattice sites' as $p \to p_c$ bears many formal similarities to the change in the 'connectivity of magnetically correlated spins' that occurs in thermally driven phase transitions as $T \to T_c$ (Kasteleyn and Fortuin 1969). In particular, one can define critical exponents for the relevant quantities that are singular at the percolation threshold p_c. One finds that these exponents depend on lattice dimensionality d but not on details of lattice geometry ('universality') and that the exponents are related to one another through a variety of equalities, each involving three different exponents ('three-exponent scaling laws').

The percolation problem (figure 1(*a*)) corresponds to the path $T = 0$, $p \to p_c$ of figure 1(*b*). Moreover, the point $p = p_c$ is thought to be the point at which the critical line $T_c(p)$ touches the $T = 0$ axis. Hence, it follows that at the point Q ($p = p_c$, $T = 0$) the system is undergoing a thermally driven phase transition if approached along the

† Work supported by the NSF and AFOSR.
‖ The presence of Griffiths singularities (Griffiths 1969) for all $T < T_c(p = 1)$ will be assumed, provisionally, not to disrupt the asymptotic behaviour of the usual magnetic singularities near $T_c(p)$.

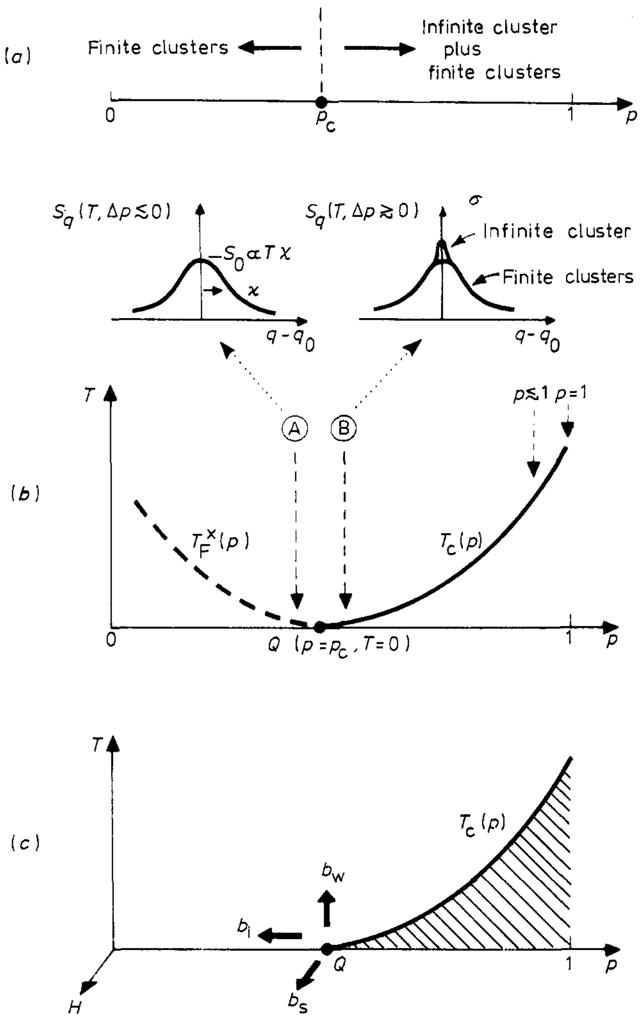

Figure 1. Schematic representations of (*a*) the pure percolation problem, (*b*) phenomena anticipated for thermally driven phase transitions near the percolation threshold, and (*c*) the phase diagram near the point Q ($p = p_c$, $T = 0$), indicating the coexistence surface (shown shaded) and the critical line $T_c(p)$, which together serve to define the strong, weak and independent scaling directions corresponding to the scaling powers b_s, b_w and b_i, respectively.

path $p = p_c$, $T \to 0$ and a lattice-connectivity driven percolation transition if approached along the path $T = 0$, $p \to p_c$. One might therefore anticipate novel phenomena to occur near the point Q. In particular, since both thermally driven phase transitions and the percolation transition are described by homogeneous functions, one might anticipate the possibility that the point Q will have scaling properties analogous to those at higher-order critical points (Riedel 1972, Hankey *et al* 1973).

The purpose of this work is to present a scaling treatment of the point Q ($p = p_c$, $T = 0$) and, further, to explore the consequences of an additional assumption concerning cluster connectivity that provides quantitative predictions for scaling powers, and hence for critical exponents and scaling functions. Independently, Stauffer (1975) has proposed a scaling hypothesis for the point Q, and his work has been extended by Lubensky (1976).

Both authors limit their discussion to the region $p \gtrsim p_c$ and both make the assumption that the two-exponent equality $d\nu = 2 - \alpha$ is valid. The treatment presented below does not assume $d\nu = 2 - \alpha$, and applies straightforwardly for $p \lesssim p_c$ as well as for $p \gtrsim p_c$. It leads to reasonably good agreement with the data on the quasi-two-dimensional magnet $Rb_2Mn_pMg_{1-p}F_4$ (Birgeneau *et al* 1976), in contrast to the Stauffer and Lubensky theories.

Scaling Theory. We begin by considering the phase diagram shown in figure 1. To define the scaling axes, we identify 'strong', 'weak' and 'independent' directions, as shown in figure 1(*c*) (Griffiths and Wheeler 1970). The scaling hypothesis for the two-spin correlation function $C_2 \equiv \langle s_0 s_r \rangle_T$ is that there exist four numbers b_s, b_w, b_i and b_r such that, sufficiently near the critical point, C_2 is a generalized homogeneous function (GHF) in all four of its arguments:

$$C_2(\lambda^{b_s}H, \lambda^{b_w}T, \lambda^{b_i}\Delta p, \lambda^{b_r}r) = \lambda C_2(H, T, \Delta p, r), \tag{1}$$

where $\Delta p \equiv p - p_c$. Henceforth, we set $H = 0$ for the sake of simplicity; scaling expressions for $H \neq 0$ are readily obtained following the same steps that lead to the $H = 0$ expressions below. From (1) it follows that the spatial Fourier transform of C_2 is a GHF with scaling power $1 + db_r$ (Hankey and Stanley 1972)

$$S(\lambda^{b_w}T, \lambda^{b_i}\Delta p, \lambda^{-b_r}q) = \lambda^{1+db_r}S(T, \Delta p, q) \tag{2a}$$

and that the inverse correlation length

$$\kappa \equiv \left(\int r^2 C_2(r)\,\mathrm{d}r \Big/ \int C_2(r)\,\mathrm{d}r\right)^{-1/2}$$

is a GHF with scaling power $-b_r$:

$$\kappa(\lambda^{b_w}T, \lambda^{b_i}\Delta p) = \lambda^{-b_r}\kappa(T, \Delta p). \tag{2b}$$

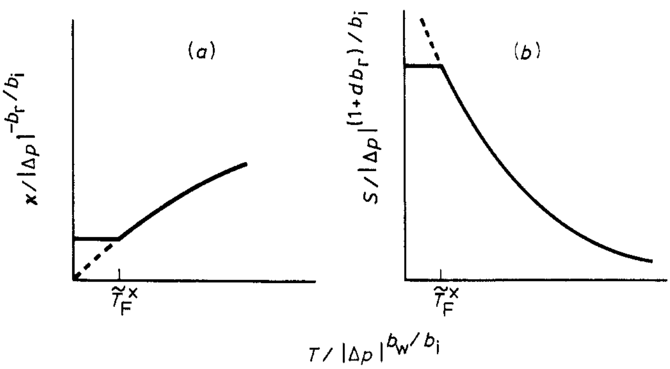

Figure 2. Scaling functions predicted by equation (3) for (*a*) the inverse correlation length κ, and (*b*) the structure factor S. The singular behaviour shown breaks down when the magnetic correlations exceed in range the characteristic size of the finite clusters; this occurs at the temperature $\tilde{T}_F^{\times} \equiv T_F^{\times}/(\Delta p)^{b_w/b_i}$.

On setting $\lambda = |\Delta p|^{-1/b_i}$ in (2*a*) and (2*b*), we obtain the scaling functions for the structure factor (figure 2(*a*))

$$\frac{S}{|\Delta p|^{(1+db_r)/b_i}} = f(\tilde{T}) \tag{3a}$$

and inverse correlation length (figure 2(*b*))

$$\frac{\kappa}{|\Delta p|^{-b_r/b_i}} = g(\tilde{T}). \qquad (3b)$$

Here $\tilde{T} \equiv T/|\Delta p|^{b_w/b_i}$ denotes the temperature scaled with respect to Δp.

Ansatz. To make quantitative predictions, one needs numerical values for the scaling powers b_x. The scaling hypothesis itself cannot predict values of the scaling powers, and therefore additional assumptions are necessary. We shall see that the b_x can be evaluated (and that the results lead to plausible predictions) by assuming that, at percolation, magnetic correlations spread through the incipient 'infinite cluster' along a path that is a self-avoiding walk (SAW). This *Ansatz* is consistent with statements in the literature of the sort that, at percolation, 'SAWs represent the most economical way the fluid can spread across the medium' (Shante and Kirkpatrick 1971). In fact, an SAW model has been proposed by Birgeneau *et al* (1976) to describe the temperature dependence of κ in $Rb_2Mn_pMg_{1-p}F_4$.

We summarize below the evidence that persuades us of the plausibility of the *Ansatz* for a two-dimensional system. Even if the *Ansatz* itself is not valid, the arguments presented below suggest that its predictions are a good first approximation toward a quantitative description of thermally driven phase transitions near the percolation threshold.

(*a*) Intuitive argument. That order propagates along paths that are SAWs in the $p \simeq p_c$ clusters is at least plausible on examination of computer simulations of finite clusters (c.f. figure 3). The main feature characterizing the large clusters (which dominate the critical scattering) is that they have a high degree of 'ramification' or 'stringiness'.

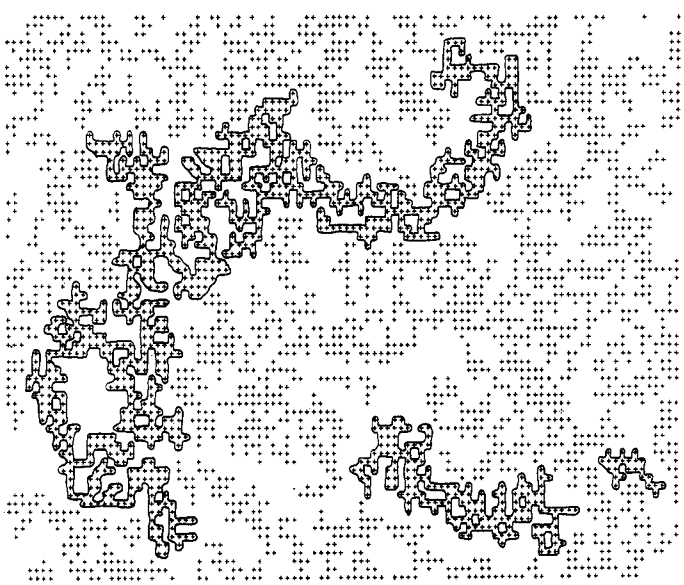

Figure 3. Computer-generated picture of the diluted square lattice for $p = 0{\cdot}53$ ($p_c \simeq 0{\cdot}59$). Here the plus symbol represents the presence of a magnetic site. All sites belonging to clusters of less than 5 sites have been eliminated as an aid to recognizing the shape of the larger clusters, which dominate the scattering. Note that most paths along which order can propagate between two distant points in the same cluster are SAWs, thereby supporting the plausibility of the *Ansatz* presented in the text.

Moreover, if one examines the possible paths along which correlations might spread from one point in a large cluster to another distant point in the same cluster, one is persuaded that the overwhelming majority of such paths are SAWs. The fact that small 'clumps' of spins which are highly connected do appear does not vitiate the above conclusion, for the spins in the clumps should order at a relatively large temperature and hence play the role of 'renormalized' spins in the critical region.

(*b*) Features of cluster connectivity. If the clusters at percolation had the full connectivity of a two-dimensional lattice, then one would expect that

$$N_{\mathrm{p}} \sim \xi_{\mathrm{p}}^{d_{\mathrm{p}}} \tag{4a}$$

with effective dimensionality† $d_{\mathrm{p}} = 2$, while if the clusters were highly ramified (as is an SAW), one would expect $d_{\mathrm{p}} < 2$. As $p \to p_{\mathrm{c}}$, $N_{\mathrm{p}} \sim |p - p_{\mathrm{c}}|^{-\gamma_{\mathrm{P}}}$ and $\xi_{\mathrm{p}} \sim |p - p_{\mathrm{c}}|^{-\nu_{\mathrm{P}}}$; hence the effective dimensionality of the percolation clusters is given in terms of the critical exponents of the percolation problem as

$$d_{\mathrm{p}} = \gamma_{\mathrm{p}}/\nu_{\mathrm{p}}. \tag{4b}$$

The effective dimensionality d_{p}, as determined by standard methods, is indeed substantially lower than two:

(i) Series expansions (Dunn *et al* 1975) find

$$d_{\mathrm{p}} = 1{\cdot}78 \pm 0{\cdot}04. \tag{5a}$$

(ii) Monte Carlo simulations (Mandelbrot 1976) find

$$d_{\mathrm{p}} = 1{\cdot}78 \pm 0{\cdot}02 \tag{5b}$$

(iii) Numerical studies on clusters of all sizes on a square lattice ($p_{\mathrm{c}} = 0{\cdot}59$) show that, when $p = 0{\cdot}55$, the number of spins in a cluster is roughly proportional to the RMS diameter of that cluster raised to the power 1·76 (Leath 1976).

(*c*) Features of SAW connectivity. The SAW problem corresponds to the $n = 0$ limit of the n-vector model (de Gennes 1972). For $d = 2$, the critical exponent $\eta_0 = 2 - \gamma_0/\nu_0$ is approximately $\frac{2}{9}$; the subscript zero denotes the $n = 0$ limit. Hence the effective dimensionality of an '$n = 0$ lattice' (i.e. a lattice on which only SAW paths have non-zero weight) is

$$d_0 \simeq 1{\cdot}78. \tag{6}$$

The agreement between (5) and (6) supports the *Ansatz*.

(*d*) Connection with other treatments of the problem. Features of the SAW problem arise in the treatment of the randomly dilute ferromagnet both by series methods and by renormalization group methods. The largest power of p in each term of the high-temperature series expansion for the randomly dilute ferromagnet is equal to the corresponding coefficient in the series expansion for the $n = 0$ model. Although the largest power of p dominates only in the 'unphysical' domain $p > 1$, this result is nevertheless intriguing. Similarly, one of the fixed points predicted by the renormalization group analysis of the same model (Aharony *et al* 1976) is the $n = 0$ fixed point. The $n = 0$ fixed point is in a physically inaccessible region for $p \simeq 1$, but for $p \simeq p_{\mathrm{c}}$ this fixed point could become accessible. That the $n = 0$ model arises in these other treatments of the same problem suggests that SAWs may play some role in the actual behaviour.

† The 'effective dimensionality' defined here is almost certainly the 'fractal dimensionality' treated by Mandelbrot (1975).

$p \leqslant p_c$. From this *Ansatz* (independent of scaling) we can describe the crossover curve $T_F^{\times}(p)$ (defined to be the temperature below which the spins belonging to a characteristic finite cluster are essentially ordered). As $T \to T_F^{\times}(p)$ along a path such as path A in figure 1(*b*), the RMS diameter of the SAW that describes the propagation of order among the spins in the cluster approaches the RMS diameter of the cluster itself. The former quantity is proportional to L^{ν_0} where L is the number of links in an SAW, while the latter is proportional to ξ_p. Hence

$$L^{\nu_0} \sim \xi_p. \tag{7}$$

For $d = 2$, $\nu_0 \simeq 0{\cdot}75$ (Domb 1969). To relate Δp to T, we note that $\xi_p \sim |p - p_c|^{-\nu_p}$, and since magnetic correlations spread along an SAW with a one-dimensional connectivity, $L \sim T^{-1}$ for $n > 1$ and $L \sim \exp(J/kT)$ for $n = 1$ (Stanley 1969). Therefore, for $n \neq 1$, the line $T_F^{\times}(p)$ is parametrized by the equation

$$T_F^{\times}(p) \sim |\Delta p|^{\phi}, \tag{8a}$$

with $\phi = \nu_p/\nu_0$.

If, moreover, scaling holds at the point Q, then

$$\phi = b_w/b_i = \nu_p/\nu_0. \tag{8b}$$

We can go further, since in the present theory b_i and b_r are the same as for the pure percolation problem (the $T = 0$ axis). Since b_i is the scaling power of the non-ordering field (Δp) in the percolation problem, and $\nu_p = -b_r/b_i$, equation (8*b*) identifies b_w as the scaling power of the non-ordering field (T) in the $n = 0$ problem. Thus, behaviour near point Q is a mixture of thermally driven and geometrically driven phenomena, with the thermally driven phenomena being described quantitatively by the scaling power b_w of the non-ordering field in the SAW problem, and the geometrically driven phenomena being described by the scaling power b_i of the non-ordering field in the percolation problem.

From the estimates for percolation and SAW exponents, it is straightforward to obtain numerical values for all the scaling powers b_x; to two significant figures we find

$$b_s = 8{\cdot}5, \quad b_w = 6{\cdot}0, \quad b_i = 3{\cdot}5 \quad \text{and} \quad b_r = -4{\cdot}5. \tag{9}$$

From (9) we readily obtain numerical predictions for the critical exponents characterizing point Q (c.f. table 1), including the quantities that appear in the scaling functions of equation (3) (c.f. figure 2).

Certain of the predictions can be subjected to checks. Firstly, the theory predicts that the length scaling powers of the percolation and the $n = 0$ problems be identical, and in fact they are. According to the best numerical estimates of equations (5) and (6) above: $b_r = -1/(d - 2 + \eta)$, where $\eta_p = 2 - d_p$ and $\eta_0 = 2 - d_0$. Secondly, the scaling powers for the 'ordering field' are predicted to be identical for both problems, which they are to within the errors inherent in the numerical methods used for their evaluation. Thirdly, although, as discussed by Birgeneau *et al* (1976), explicit comparison with their experiments on $Rb_2Mn_pMg_{1-p}F_4$ is complicated by several factors, including finite size and spin–space crossover ($n = 3 \to n = 1$) effects, their experiments nevertheless do favour the SAW *Ansatz* over the alternative theories. In particular, they have shown that for $p = 0{\cdot}56$ the inverse correlation length follows the power law $\kappa \sim \xi_1^{-0.75 \pm 0.01}$, where ξ_1 is the one-dimensional longitudinal correlation length including the anisotropy explicitly. However, a more exhaustive experimental test of the present approach will have to await new experiments on a system with p very close to p_c and with minimal anisotropy effects.

Table 1. Critical exponents predicted by scaling theory for the point Q ($p = p_c$, $T = 0$) of figure 1. The exponents are given their usual names, with an additional bar to denote the fact that they refer to a competing higher-order point Q, and with a subscript to denote the path of approach to the point Q: w denotes a 'weak' direction (a curve that always remains above the curve $T = |\Delta p|^{\phi}$) and i denotes an 'independent' direction (a path of approach that always remains below the curve $T = |\Delta p|^{\phi}$). The general scaling expressions hold independent of the *Ansatz*. Comparison between the numerical predictions and experimental data is discussed in the text.

Exponent	General scaling expression	Numerical value predicted by *Ansatz* for $d = 2$ (c.f. equation(9))	Numerical value § predicted if $\phi = 2$ (Stauffer 1975)	Numerical value predicted if $\phi = 1{\cdot}1$ (Lubensky 1976)
ϕ	b_w/b_i	1·7	2	1·1
ν_i	$-b_r/b_i$	1·3	1·3	1·3
ν_w	$-b_r/b_w$	0·75	0·65	1·2
γ_i	$-(1 + db_r)/b_i$	2·3	2·3	2·3
γ_w	$-(1 + db_r)/b_w$	1·3	1·15	2·1
α_i	$-(1 + db_r + 2b_s - 2b_w)/b_i$	0·86	0·86	0·86
α_w	$-(1 + db_r + 2b_s - 2b_w)/b_w$	0·5	0·43	0·78

§ These exponents are defined with respect to the scaling axes introduced by Stauffer.

$\underline{p \geq p_c}$. Now consider path B of figure 1(*b*) for which $p \gtrsim p_c$. In addition to the finite clusters, a small fraction P_p of the sites belong to an infinite cluster; the structure factor now displays an additional sharp central peak (c.f. figure 1(*b*)). The finite clusters above p_c are analogous to the finite clusters below p_c, and therefore the $p \lesssim p_c$ arguments also hold for $p \gtrsim p_c$. However, the infinite cluster gives rise to two-dimensional long-range order at some temperature $T_c(p)$. To describe the behaviour in the infinite cluster, we first consider $T \gg T_c(p)$: at sufficiently large T, the correlations will not be two-dimensional in nature because the correlation length ξ_n will not be sufficiently large to recognize the fact that the infinite cluster has true two-dimensional connectivity. In fact, at high temperature, the magnetic correlations spread along the zig-zag paths with essentially one-dimensional correlations. At some temperature $T^{\times}_{\infty}(p)$, ξ_n becomes comparable to $l(p)$, the node-to-node distance† (measured along the zig-zag path connecting them), and the system begins to display two-dimensional correlations (Lubensky 1976, de Gennes 1976). Thus $T^{\times}_{\infty}(p)$ is a crossover temperature between SAW behaviour and two-dimensional behaviour in the infinite lattice. For $T > T^{\times}_{\infty}(p)$, $\xi_n \sim 1/T$. As $T \to T^{\times}_{\infty}(p)$ from above, the correlation length ξ_n approaches $l(p)$ and we have $l(p) \sim 1/T^{\times}_{\infty}(p)$. The p-dependence of $l(p)$ is obtained from the fact that for $T > T^{\times}_{\infty}(p)$ the correlations spread along paths that are SAWs, and hence, in analogy to (7), $[l(p)]^{\nu_0} \sim \xi_p$, where $\xi_p \sim |p - p_c|^{-\nu_P}$ is the distance between nodes 'as the crow flies'. If we assume that $\hat{\xi}_p \sim \xi_p$, then

$$T^{\times}_{\infty}(p) \sim |\Delta p|^{\nu_P/\nu_0}. \tag{10}$$

Comparing (8) and (10), the above assumption implies that $T^{\times}_{\infty}(p)$ has the same Δp-dependence, and hence the same shape as $T^{\times}_{F}(p)$. The same assumptions show that $T_c(p)$ is also described by the crossover exponent ν_p/ν_0.

The results presented here have been tested by comparison with existing numerical calculations and with experimental data on thermally driven phase transitions near the

† A node is a point in the lattice having three or more independent paths to infinity.

percolation threshold. Further, it would be desirable (i) to test other exponent predictions of the theory (table 1), (ii) to check the scaling function predictions that follow from (1) (c.f., for example, equation (3) and figure 2), (iii) to see whether there is evidence favouring the *Ansatz* for $d \neq 2$ (for $d = 3$, the predictions are $\phi = 1{\cdot}58$, $\nu_w = 0{\cdot}6$ and $\gamma_w = 1{\cdot}2$), (iv) to test the predictions concerning the shapes of the curves $T_c(p)$, $T_F^{\times}(p)$ and $T_{\infty}^{\times}(p)$.

In summary, then, the scaling theory should be valid if Q is like other higher-order critical points. A further assumption concerning cluster connectivity near the percolation threshold leads to quantitative predictions for both critical exponents and scaling functions. The crossover exponent is predicted to take the same value for all $n > 1$, which is rather different from the situation for $p = 1$ where critical phenomena depend strongly upon n; on the other hand, the behaviour for $n = 1$ is drastically different from that for $n > 1$, so that spin-dimensionality crossover effects may be expected to play a significant role near the percolation threshold.

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