VOLUME 28, NUMBER 11

Finite-size scaling for directed self-avoiding walks

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A directed self-avoiding walk model is solved exactly for a finite cylinder geometry where the cylinder's axis is parallel to the directed axis of the walk. The finite-size scaling behavior of the longitudinal and transverse correlation lengths is examined. Although the infinite system has a continuous transition, one of the scaling variables for the finite system varies exponentially with the cylinder circumference, which is reminiscent of finite-size effects at first-order transitions in scalar-spin systems.

Finite-size scaling theory^{1,2} is a topic of appreciable theoretical interest (see Ref. 3 for a review). Precise estimates of critical exponents for various two-dimensional lattice models have been obtained by applying this theory to transfer-matrix calculations (see Ref. 4 for a review). The finite-size behavior at normal critical or continuous transition points can be derived in a simplified way^{5,6} by regarding the inverse lengths $1/L_i$ as extra scaling fields. For example, for the order parameter *m* of a spatially anisotropic two-dimensional system on an $L_{\parallel} \times L_{\perp}$ lattice, one obtains

$$m(T;L_{\parallel},L_{\perp}) \approx m_{\infty}(T)M\left[\frac{L_{\parallel}}{\xi_{\parallel,\infty}(T)},\frac{L_{\perp}}{\xi_{\perp,\infty}(T)}\right]$$
(1)

as the reduced temperature $t = (T_c - T)/T_c \rightarrow 0^+$ at ordering field H = 0: Here m_{∞} , $\xi_{\parallel,\infty}$, and $\xi_{\perp,\infty}$ are the bulk order parameter and correlation lengths, which vary as t^{β} , $t^{-\nu_{\parallel}}$, and $t^{-\nu_{\perp}}$, respectively, near the bulk critical temperature $T = T_c$. We shall refer to (1) as a strong scaling hypothesis. More elaborate renormalization-group analysis⁷ suggests that for, say, the case $L_{\parallel} = L_{\perp} = L$, L should probably be regarded not as the inverse of a standard scaling field but as a renormalization-group flow parameter. The leading scaling relation (1) has been confirmed in many cases,³ although there are difficulties⁸ with the systematic analysis of correction terms.

Recently, a scaling theory of finite-size effects at *first-order* transitions has been developed.^{9,10} In two dimensions, it prescribes that the two arguments of relation (1) be replaced by the single scaling variable combination $L_{\parallel}L_{\perp}/l_{H}^{2}$, where

$$l_{H}(T) = |k_{G}T/m_{\infty}(T)H|^{1/2}$$
(2)

is a "phase persistence length" whose divergence at $H \rightarrow 0$ for $T < T_c$ fixed reflects the occurrence of long-range order in the correlation functions that distinguish the two, coexisting, oppositely magnetized phases at the first-order transition.⁹ In addition, it is found¹⁰ that in the limit $L_{\parallel} >> L_{\perp}$ (where the lattice becomes a "strip"), a new length, $l_{\parallel}(L_{\perp},T)$, also enters the finite-size scaling forms. Fluctuations break the ferromagnetic strip at H=0 into segments of oppositely magnetized domains: l_{\parallel} represents the characteristic longitudinal extent of one of these single-phase domains. As such, it is proportional to the finite-strip longitudinal correlation length at the bulk first-order transition and varies^{10, 11} as

$$l_{\parallel}(L_{\perp},T) \sim e^{L_{\perp}\sigma(T)}$$
, (3)

where $\sigma(T) \equiv \Sigma(T)/k_B T$ is the reduced surface tension of the transverse domain walls. Thus, a new argument $L_{\parallel}/l_{\parallel}(L_{\perp})$, which depends exponentially on L_{\perp} , must be included in the finite-size scaling relation for the first-order transition, which may then be written

$$m(T,H;L_{\parallel},L_{\perp}) \approx m_{\infty}(T)\tilde{M}\left\{\frac{L_{\parallel}L_{\perp}}{[l_{H}(T)]^{2}},\frac{L_{\parallel}}{l_{\parallel}(L_{\perp},T)}\right\}$$
(4)

as $H \rightarrow 0$ at $T < T_c$ fixed. For further details and a discussion of the difficulties associated with the derivation of finite-size scaling for first-order transitions from renormalization-group analyses,^{9,12,13} the reader should consult Ref. 10.

By adopting a more general notation in which $\xi_{\parallel,\infty}$ and $\xi_{\perp,\infty}$ are taken to represent the bulk correlation lengths in the case of a continuous transition but the phase persistence lengths in the case of a first-order transition, one can subsume both scaling relations (1) and (4) under the single relation

$$m(T,H;L_{\parallel},L_{\perp}) \approx m_{\infty}(T) X \left(\frac{L_{\parallel}}{\xi_{\parallel,\infty}}, \frac{L_{\perp}}{\xi_{\perp,\infty}}, \frac{L_{\parallel}}{l_{\parallel}(L_{\perp})} \right) .$$
(5)

We shall refer to (5) as a *weak* scaling hypothesis: Note, in particular, that it generalizes the usual finite-size scaling relation (1) to include the length $l \parallel (L_{\perp}) \sim e^{L_{\perp}\sigma}$. For continuous bulk transitions, this new length is not normally expected, but it does in fact arise in the model that will now be discussed.

Our model is a directed self-avoiding walk on a finite square lattice of $L_{\parallel} \times L_{\perp}$ sites¹⁴⁻¹⁸. This problem was first studied (for infinite lattices) by Fisher and Sykes,¹⁴ and for finite lattices by Redner.¹⁵ It is a self-avoiding walk subject to the additional constraint that steps along one "directed" axis (taken here to be the x axis) may be in only one direction (here, $+\hat{x}$). We consider periodic boundary conditions in the y direction, so that the walk is actually on a cylinder of length L_{\parallel} and circumference L_{\perp} . (Here and henceforth we assume the lattice constant a to be unity.) Assign weights z_{\parallel} , z_+ , and z_- , respectively, to every horizontal $(+\hat{x})$, upward $(+\hat{y})$, and downward $(-\hat{y})$ step, and let $G_{n+n-}^{(N)}(L_{\parallel},L_{\perp})$ denote the number of N-step walks which start at the origin (x=0, y=0) and have n_+ upward and n_- downward steps.

Consider first the case $L_{\parallel} = \infty$. Then the generating function for these walks is^{14, 18, 19}

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$$G(z_{\parallel}, z_{+}, z_{-}; \infty, L_{\perp}) \equiv \sum_{N, n_{+}, n_{-}} G_{n_{+}n_{-}}^{(N)}(\infty, L_{\perp}) z_{\parallel}^{N-n_{+}-n_{-}} z_{+}^{n_{+}} z_{-}^{n_{-}} = H[1 + z_{\parallel}H + (z_{\parallel}H)^{2} + (z_{\parallel}H)^{3} + \cdots] = H/(1 - z_{\parallel}H) ,$$
(6)

where H denotes the generating function for a walk parallel to the y axis:

$$H(z_{+}, z_{-}; L_{\perp}) = 1 + (z_{+} + z_{+}^{2} + \cdots + z_{+}^{L_{\perp}-1}) + (z_{-} + z_{-}^{2} + \cdots + z_{-}^{L_{\perp}-1}) = 1 + \frac{z_{+} - z_{+}^{L_{\perp}}}{1 - z_{+}} + \frac{z_{-} - z_{-}^{L_{\perp}}}{1 - z_{-}} .$$
(7)

The total number of N-step walks, ${}^{14} c_N(\infty, L_1)$, is then generated from the "susceptibility"

$$\chi(z;\infty,L_{\perp}) = G(z,z,z;\infty,L_{\perp}) = \sum_{N=0}^{\infty} c_N(\infty,L_{\perp}) z^N$$
$$= (1+z-2z^{L_{\perp}})/(1-2z-z^2+2z^{L_{\perp}+1}) \quad . \tag{8}$$

(See Refs. 20 and 21 for discussions of the analogy between the self-avoiding walk problem and ferromagnetic models exhibiting continuous transitions.) For the infinite lattice $(L_{\perp} = \infty)$, the singularity of χ nearest the origin is a simple pole at

$$z = z_c = \sqrt{2} - 1 \quad , \tag{9}$$

which represents a bulk critical point near which $\chi(z;\infty,\infty)$ behaves as $(z_c - z)^{-\gamma}$ with $\gamma = 1$. The mean horizontal displacement of N-step walks is defined by

$$\langle R_{\parallel}^{(N)}(\infty, L_{\perp}) \rangle \equiv c_N^{-1} \sum_{n_+, n_-} (N - n_+ - n_-) G_{n_+ n_-}^{(N)}$$
, (10)

in terms of which one then defines the longitudinal correlation length as

$$\xi_{\parallel}(z;\infty,L_{\perp}) = \left(\sum_{N=0}^{\infty} c_N \langle R_{\parallel}^{(N)} \rangle z^N\right) / \left(\sum_{N=0}^{\infty} c_N z^N\right)$$
$$= z \left(\frac{\partial \ln G}{\partial z_{\parallel}}\right)_{z_{\parallel}=z_{\perp}=z_{\perp}=z_{\perp}}.$$
(11)

Thus, from (6) and (8) one obtains the simple result

$$\xi_{\parallel}(z;\infty,L_{\perp}) = z\chi(z;\infty,L_{\perp}) \quad . \tag{12}$$

Defining $t = (z_c - z)/z_c$, one then has, in the bulk system,

$$\xi_{\parallel}(z;\infty,\infty) \approx \frac{1}{2}t^{-\nu_{\parallel}} \text{ with } \nu_{\parallel} = 1$$
 (13)

The (squared) transverse correlation length is similarly defined in terms of the mean-square transverse displacement of N-step walks,

$$\langle [R_{\perp}^{(N)}(\infty, L_{\perp})]^2 \rangle \equiv c_N^{-1} \sum_{\substack{n_+, n_- \\ n_+, n_-}} (n_+ - n_-)^2 G_{n_+ n_-}^{(N)} , \quad (14)$$

as

$$\xi_{\perp}^{2}(z;\infty,L_{\perp}) = \left(\sum_{N=0}^{\infty} c_{N} \langle (R_{\perp}^{(N)})^{2} \rangle z^{N} \right) / \left(\sum_{N=0}^{\infty} c_{N} z^{N} \right)$$
$$= \hat{D}_{\perp} G(z_{\parallel}, z_{\perp}, z_{\perp}, ;\infty, L_{\perp}) \quad , \tag{15}$$

where

$$\hat{D} = (1/\ell) \left[\frac{1}{\ell^2} \left[\frac{\partial}{\partial t} - \frac{\partial}{\partial t} \right]^2 + 2 \frac{1}{\ell^2} \frac{\partial}{\partial t} \right]^2$$

$$\hat{D}_{\perp}f = (1/f) \left[z^2 \left(\frac{\partial}{\partial z_{+}} - \frac{\partial}{\partial z_{-}} \right)^2 + 2z \frac{\partial}{\partial z_{+}} \right] f|_{z_{\parallel} - z_{+} - z_{-} - z_{-}}$$
(16)

[Note that according to the convention adopted here, a walk with a total of, say, $2L_{\perp}-1$ upward steps and no downward steps is regarded as having a transverse displacement of $2L_{\perp}-1$ from its origin (not 1, as measured from the shortest path back to the origin). This convention is mathematically convenient and, in the limit $L_{\perp} \rightarrow \infty$, reduces to the usual bulk definition of transverse displacement.] Thus one readily finds

$$\xi_{\perp}^{2}(z;\infty,L_{\perp}) = [\xi_{\parallel}(z;\infty,L_{\perp}) + 1]D_{\perp}H(z_{\perp},z_{\perp};L_{\perp}) , \quad (17)$$
where

where

$$\hat{D}_{\perp}H(z_{+},z_{-};L_{\perp}) = 2z/(1-z)^{2} + O(L_{\perp}^{2}z^{L_{\perp}}) \quad . \tag{18}$$

Therefore, in the bulk system, one has

$$\xi_{\perp}^{2}(z;\infty,\infty) \approx \frac{1}{2z_{c}} t^{-2\nu_{\perp}} \text{ with } \nu_{\perp} = \frac{1}{2} .$$
 (19)

Now let us examine the behavior of these results (12) and (17) for the correlation lengths when L_{\perp} is finite. In that case, (8) implies that ξ_{\parallel} and ξ_{\perp} still diverge (again with exponents $\nu_{\parallel} = 1$, $\nu_{\perp} = \frac{1}{2}$), but at a shifted critical point

$$z = z_0(L_{\perp}) = z_c [1 + 2^{-1/2} z_c^{L_{\perp}} + O(L_{\perp} z_c^{2L_{\perp}})] \quad .$$
 (20)

It follows that $at z = z_c$, ξ_{\parallel} diverges exponentially with L_{\perp} :

$$\xi_{\parallel}(z_c;\infty,L_{\perp}) \approx 2^{-1/2} z_c^{-L_{\perp}} .$$
 (21)

Therefore, as the finite system approaches bulk criticality $(z \rightarrow z_c^{-}, L_{\perp} \rightarrow \infty)$, this new length scale appears in addition to the usual diverging length scales set by the system dimensions $L_{\parallel,\perp}$ and the bulk correlation lengths $\xi_{\parallel,\perp}(z;\infty,\infty)$. Accordingly, in order to cast the scaling form of ξ_{\parallel} near bulk criticality in the same form as the scaling hypothesis (5), it proves convenient to set $c = -\ln z_c > 0$ and define an exponentially divergent length

$$l_{\parallel}(L_{\perp}) \equiv e^{cL_{\perp}} = z_c^{-L_{\perp}} \sim \xi_{\parallel}(z_c; \infty, L_{\perp}) \quad .$$
 (22)

From (12) and (8), the exact result for ξ_{\parallel} can then be written asymptotically as

$$\xi_{\parallel}(z;\infty,L_{\perp}) \approx \frac{1}{2t} W[2tl_{\parallel}(L_{\perp})] \quad , \tag{23}$$

where

$$W(v) \equiv v/\sqrt{2} + v) \quad . \tag{24}$$

By virtue of (13), this is equivalent to

$$\xi_{\parallel}(z;\infty,L_{\perp}) \approx \xi_{\parallel}(z;\infty,\infty) W \left(\frac{l_{\parallel}(L_{\perp})}{\xi_{\parallel}(z;\infty,\infty)} \right) .$$
(25)

One can now recognize (25) as a special form of the weak scaling hypothesis (5), where for this problem the scaling

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function X(x,y,z) is reduced to a single-variable function W(x/z) at $L_{\parallel} \rightarrow \infty$. However, (25) does *not* have the form of the strong scaling hypothesis (1) that one might expect to hold for this system with a continuous bulk transition. Instead, the scaling form (25) involves the additional length $l_{\parallel}(L_{\perp})$ which varies asymptotically with L_{\perp} in a manner similar to the longitudinal correlation length (3) for first-order systems. [Clearly, by virtue of (17) and (18), the same conclusions apply to ξ_{\perp} .] Notice that the strong scaling hypothesis for the correlation lengths in the case $L_{\parallel} = \infty$ can be rewritten

$$\xi_i(t;\infty,L_\perp) \approx L_\perp^{\nu_i/\nu_\perp} Y(L_\perp t^{\nu_\perp}), \quad i = || \text{ or } \perp \ , \qquad (26)$$

whereas (22) and (23) imply that for this directed selfavoiding walk model,

$$\xi_{\parallel}(z;\infty,L_{\perp}) \approx e^{cL_{\perp}} \tilde{Y}(e^{cL_{\perp}}t^{\nu_{\parallel}}) \quad , \tag{27}$$

with a similar result for ξ_{\perp} . This anomalous dependence on L_{\perp} is clearly a consequence of the extreme asymptotic anisotropy of the model, although it is worth noting that for another anisotropic problem, namely, directed percolation (see Ref. 22 for a review), no discrepancies were observed when the strong scaling hypotheses (26) were employed in numerical calculations.^{22,23}

The behavior for L_{\parallel} finite, which we now outline briefly, is similar. The generating function (6) becomes

$$G(z_{\parallel}, z_{+}, z_{-}; L_{\parallel}, L_{\perp})$$

= $H[1 + z_{\parallel}H + (z_{\parallel}H)^{2} + \dots + (z_{\parallel}H)^{L_{\parallel}-1}]$
= $H[1 - (z_{\parallel}H)^{L_{\parallel}}]/(1 - z_{\parallel}H)$. (28)

whence ξ_{\parallel} defined as in (11) is found to be

$$\xi_{\parallel}(z;L_{\parallel},L_{\perp}) = \xi_{\parallel}(z;\infty,L_{\perp}) - \frac{L_{\parallel}(zH_{0})^{L_{\parallel}}}{\left[1 - (zH_{0})\right]^{L_{\parallel}}} , \quad (29)$$

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where

$$H_0 = H(z, z; L_\perp) = (1 + z - 2z^{L_\perp})/(1 - z) \quad . \tag{30}$$

Its asymptotic form near bulk criticality is

$$\xi_{\parallel}(z; L_{\parallel}, L_{\perp}) \approx \frac{1}{2t} \tilde{W}(2tL_{\parallel}, 2tl_{\parallel})$$
(31)

with scaling function

$$\tilde{W}(u,v) \equiv W(v) - u/(e^{u/W(v)} - 1) , \qquad (32)$$

which again has the form of the weak but not the strong scaling hypothesis. The transverse correlation length is still given by (17) (but with $L_{\parallel} < \infty$), so that in the scaling region, one has

$$\xi_{\perp}^{2}(z; L_{\parallel}, L_{\perp}) \approx (1/z_{c}) \xi_{\parallel}(z; L_{\parallel}, L_{\perp}) \quad . \tag{33}$$

In summary, this simple soluble model demonstrates that the conventional finite-size scaling relation (1), which breaks down at first-order transitions,¹⁰ should also be used with caution in models with continuous transitions which exhibit anisotropic divergence of critical correlations.

ACKNOWLEDGMENTS

The authors are indebted to M. E. Fisher for valuable comments on the manuscript. Helpful discussions with him, M. Barma, and S. Redner are greatly appreciated. The financial support of the National Science Foundation (to A.M.S.) and through Grant No. DMR-81-17011 and that of the Rothschild Foundation (to V.P.) are gratefully acknowledged.

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