Boundary and finite-size effects in two-dimensional structure factors at criticality

Per Fröjdh*
Institute of Theoretical Physics, Chalmers University of Technology, S-412 96 Göteborg, Sweden
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We show how the apparent power-law scaling of classical two-dimensional structure factors in bounded domains at criticality is related to fixed and free boundary conditions on the order parameter. This enables us to predict the behavior of the corresponding apparent scaling dimensions based on a simple symmetry analysis. With the use of correlation functions from conformal field theory, our predictions are confirmed with exact calculations for multicritical Ising models. Effects of random boundary fields are also discussed.

INTRODUCTION

Finite size and boundary conditions of a system undergoing a second-order phase transition have a strong impact on the critical behavior.[1,2] In particular, structure factors for two-dimensional restricted domains exhibit so-called *apparent* scaling strongly dependent on boundary conditions.[3–7] The convergence toward bulk scaling has been shown to be very slow, so that critical exponents which can be deduced from diffraction experiments or numerical calculations on lattice models will either under- or overestimate the true bulk exponents. Still, the important question of how different boundaries exert an influence on structure factors has not been raised. Clearly, a systematic analysis of this issue is much wanted.

In this paper we explicitly show how structure factors are related to boundary conditions of a finite domain. On the one hand, the apparent dimensions will overestimate the true bulk dimensions of operators that have nonvanishing expectation values near the boundary. If, on the other hand, the expectation values are zero, the converse will be true in general. We analyze uniform boundary conditions on the order parameter. In addition, we consider effects of a random boundary field, which may play a role in some experimental systems.

Our predictions are confirmed by numerical calculations using exact correlation functions derived by conformal field theory methods for multicritical Ising models. For definiteness we have carried out the analysis for systems defined in a disk, but the predictions should also be applicable to other finite domains.

STRUCTURE FACTORS

The static structure factor $S(\mathbf{k})$ in a two-dimensional domain A is given by the Fourier transform of a correlation function $G(\mathbf{r}_1, \mathbf{r}_2)$:

$$S(\mathbf{k}) = \frac{1}{A}\int_A d^2r_1 d^2r_2\, G(\mathbf{r}_1,\mathbf{r}_2)\, e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)} . \qquad (1)$$

It is proportional to the scattering intensity in a diffraction experiment with momentum transfer $\mathbf{k}$ ($\hbar = 1$). For a translational invariant system in an infinite plane ($A = \mathbb{R}^2$), one has the standard expression

$$S_\infty(\mathbf{k}) = \int d^2r\, G(\mathbf{r})\, e^{i\mathbf{k}\cdot\mathbf{r}} . \qquad (2)$$

At the critical point, $G(\mathbf{r}) = \langle\phi(\mathbf{r})\phi(0)\rangle = |\mathbf{r}|^{-2x}$, leading to a power-law scaling

$$S_\infty(k) \sim \frac{1}{k^{2-2x}} , \qquad (3)$$

with x the scaling dimension of the scalar field ϕ.[8]

In a bounded domain, the correlation function in (1) is not a power law, but depends on size, shape, and boundaries of the system. Nonetheless $S(k)$ has often proved *almost* to scale with momentum at criticality:

$$S(k) \sim \frac{1}{k^{2-2x_{\rm app}}} \qquad (4)$$

where the apparent scaling dimension $x_{\rm app}$ depends *weakly* on k (or $\mathbf{k}$ for nonisotropic domains) and converges slowly for increasing k toward the bulk dimension x.[3–7] In order to see when such scaling is possible, we must investigate how finite size and boundaries influence bulk scaling.

BOUNDARY CONDITIONS

Consider a two-dimensional ferromagnetic spin system with a boundary. At the bulk-critical point there are two possible surface transitions corresponding to free and fixed boundary conditions on the order parameter. Without an ambient field coupling to the (one-dimensional) surface of the system, the boundary is said to be free, whereas it is fixed in an infinite, uniform boundary field. Although the boundaries are noncritical in general,[2] the boundary conditions are homogeneous in the continuum limit and thus preserved under conformal transformations.

In a field-theoretic description of the system, a local operator $\phi(\mathbf{r})$, defined such that $\langle\phi\rangle = 0$ in the bulk, may have a nonvanishing expectation value in the presence of a boundary. In a disk of unit radius, it is given by

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$$\langle\phi(r)\rangle = \frac{\mathcal{A}}{(1-r^2)^x}\,, \qquad (5)$$

with r measured from the center of the disk. This follows from conformally mapping the expectation value in a half-plane[9] to a disk.[10] For a free boundary (which preserves the underlying symmetry of the model), the amplitude $\mathcal{A}$ is nonzero for energylike operators, whereas it is forced to vanish for spinlike operators. However, a fixed boundary explicitly breaks the symmetry, leading to a nonzero value of $\mathcal{A}$ for both energy- and spinlike operators. Consequently, we must use the *connected* two-point function $\langle\phi(\mathbf{r}_1)\phi(\mathbf{r}_2)\rangle_c = \langle\phi(\mathbf{r}_1)\phi(\mathbf{r}_2)\rangle - \langle\phi(\mathbf{r}_1)\rangle\langle\phi(\mathbf{r}_2)\rangle$ as $G(\mathbf{r}_1,\mathbf{r}_2)$ in (1) in order to obtain the scaling law (4) in a bounded domain. ($\langle\phi\rangle \neq 0$ leads to an oscillating structure factor for $G = \langle\phi\phi\rangle$ and suppressed scaling.[11])

The leading contribution to a structure factor that exhibits apparent scaling is given by (3) as $k\to\infty$. This corresponds to the $r = |\mathbf{r}_1 - \mathbf{r}_2| \to 0$ limit of the correlation function $G(\mathbf{r}_1,\mathbf{r}_2)$ that governs this behavior. The disconnected part $\langle\phi\rangle\langle\phi\rangle$ is exactly known from (5) and, provided that $\langle\phi\rangle \neq 0$, adds a negative contribution to $S(k)$ of the form

$$\Delta S(k) \sim -\frac{1}{k^{2-2x}}\,\frac{\cos^2(k-\vartheta)}{k} \quad \text{as } k\to\infty, \qquad (6)$$

with ϑ a parameter depending linearly on x. Hence, this correction is one power of k less relevant than the leading order of $S(k)$. Although important to establish scaling, it does not change the asymptotics of the structure factor. One may therefore concentrate on $\langle\phi\phi\rangle$, whose small-distance behavior is given by the leading terms of the operator-product expansion (OPE)

$$\phi(\mathbf{r}_1)\phi(\mathbf{r}_2) \sim \frac{1}{r^{2x}}(\mathbb{1} + \mathcal{C}\,r^{x'}\,\phi'(\mathbf{r}_1) + \cdots), \qquad (7)$$

with $\mathcal{C}$ the coefficient (*structure constant*) for ϕ' with scaling dimension x'. [Notice that for a complex field ϕ, we can generalize (7) by replacing $\phi(\mathbf{r}_2)$ with its complex conjugate.] Using (5) and $\mathcal{B}$ as the amplitude of ϕ', one obtains

$$\langle\phi(\mathbf{r}_1)\phi(\mathbf{r}_2)\rangle = \frac{1}{r^{2x}}\left(1 + \frac{\mathcal{C}\mathcal{B}\,r^{x'}}{(1-r_1^2)^{x'}} + \cdots\right), \qquad (8)$$

as $r = |\mathbf{r}_1 - \mathbf{r}_2| \to 0$. The second term, containing the numerical factor $\mathcal{C}\mathcal{B}$, reflects the influence of the boundary and its sign controls the behavior of the apparent scaling, as will be shown in the following.

To obtain the leading correction to the scaling law in the infinite plane (3), we observe that

$$G(\mathbf{r}) = \frac{1}{A}\int_A d^2r_1\,d^2r_2\,\delta(\mathbf{r}-\mathbf{r}_1+\mathbf{r}_2)\;G(\mathbf{r}_1,\mathbf{r}_2) \qquad (9)$$

inserted in (2) reproduces the structure factor in (1). If $G(\mathbf{r}_1,\mathbf{r}_2)$ only depends on $\mathbf{r}_1 - \mathbf{r}_2$, the integral in (9) can be performed without further knowledge of the integrand. The first term of (8) fulfills this condition. By averaging the second term over small distances in the disk, we can estimate it by an effective term proportional to $r^{-2x+\bar{x}'}$. The average exponent $\bar{x}'$ must be in the range $(0,\,x')$, as $\mathbf{r}_2$ near the edge and at the center correspond to an exponent equal to 0 and x', respectively. Hence, we have

$$G(r) \approx \frac{1}{r^{2x}}\left(1 + \alpha\,\mathcal{C}\mathcal{B}\,r^{\bar{x}'} - \frac{2}{\pi}r + \cdots\right), \qquad (10)$$

as $r\to 0$, with $\alpha > 0$. The last term comes from the remaining integral and the dots represent terms of higher order than $r^{\bar{x}'}$ or r. When now comparing (10) with the bulk function r^{-2x}, we see that the correlations in the disk are governed by an effective scaling dimension $\tilde{x}$ such that

$$G(r) \approx \frac{1}{r^{2\tilde{x}}} \qquad (11)$$

at small distances, with $\tilde{x}\to x$ as $r\to 0$. For $\bar{x}' > 1$, we get $\tilde{x} < x$. However, this condition is difficult to control as our lower bound of $\bar{x}'$ is less than 1. Let us therefore restrict ourselves to the more ubiquitous case $\bar{x}' < 1$, which among others applies to the order parameters of the multicritical Ising models and the three-state Potts model. Whether $\tilde{x}$ will over- or underestimate x is then determined by the sign of $\mathcal{C}\mathcal{B}$, which is related to the boundary condition of ϕ.

APPARENT SCALING DIMENSIONS

The behavior of the apparent scaling dimension x_{app} in (4) at large momenta will now be the same as the effective scaling dimension $\tilde{x}$ at small distances, as (11) determines the Fourier transform in this region. Notice that (11) is only valid here and does not decay to zero at distances of the order of the domain size. However, as we concentrate on short distances, we can avoid such an unphysical behavior by instead extending the domain of integration to restore the long-distance decay. [This also makes the connection to the plane clearer, where the decay as $r\to\infty$ is crucial for obtaining Eq. (3).]

We also need the relation between the boundary conditions and the sign of $\mathcal{C}\mathcal{B}$. Consider for example $\phi = \sigma$ (magnetization) in a domain with a fixed boundary, and let the OPE coefficient $\mathcal{C}$ be positive (This is not a restriction as the *combination* $\mathcal{C}\mathcal{B}$ is completely determined by the correlation function and does not depend on the choice of $\mathcal{C}$.) The amplitude $\mathcal{B}$ will then measure the enhancement of the (ferromagnetically negative) energy density $\phi' = \epsilon$. In a square-lattice realization, a boundary spin σ has two parallel neighbors and a third neighbor of arbitrary orientation, consequently $\mathcal{B} > 0$. The same argument holds for $\phi = \epsilon$ and can be generalized to other operators in domains with fixed boundaries. With $\phi = \sigma$ and a free boundary, one has $\mathcal{B} < 0$, i.e., the energy density decreases at the boundary.[12] A generalization gives the same result for other spinlike operators. For energylike operators and a free boundary, on the other hand, we have the same result as for a fixed boundary. This follows from that $\langle\phi\phi\rangle$ is the same for fixed and free boundary conditions in this case. Thus, one can summarize both fixed and free boundary conditions in the following way: $\langle\phi\rangle \neq 0$ yields $\mathcal{CB} > 0$, and $\langle\phi\rangle = 0$ yields $\mathcal{CB} < 0$.

We can now draw the main conclusion of this analysis, namely how the boundary conditions govern the apparent scaling dimension $x_{\rm app}$. For *large momenta* we have that *$x_{\rm app} > x$ for an operator ϕ in a domain with a boundary condition such that $\langle\phi\rangle \neq 0$. For $\langle\phi\rangle = 0$, $x_{\rm app} < x$.* Hence, from a simple symmetry analysis of the boundary conditions we can predict whether $x_{\rm app}$ under- or overestimates x at large momentum transfers k.

At the other extreme, $k = 0$, we can directly see that $x_{\rm app} = 1$. This follows from the Gaussian shape of $S(k)$ at small k, obtained from an expansion of (1). By connecting the two extremes with a smooth function $x_{\rm app}$, the generic types of apparent scaling are shown in Fig. 1 for the case $x < 1$. (For $x > 1$, the structure factor is nonsingular in the thermodynamic limit, and for $x = 1$, it is expected to diverge logarithmically, as has been observed for an infinite cylinder.[5]) The upper curve ($\langle\phi\rangle \neq 0$) will always give $x_{\rm app} > x$, whereas for the lower curves ($\langle\phi\rangle = 0$) there is a crossover to $x_{\rm app} < x$. Moreover, the explicit calculations of $x_{\rm app}$ below suggest that $x_{\|} < 1$ gives an immediate transition to $x_{\rm app} < x$, while for $x_{\|} > 1$ the transition does not occur until k is near the asymptotic regime. Here $x_{\|}$ is the surface exponent that controls the decay of the correlations along the boundary. As the transition must occur for a finite value of k, which sets the length scale at which correlations in the domain are probed, correlations in a finite part of the domain along the boundary are affected by the surface exponent. Hence, the effective scaling dimension sensed by $x_{\rm app}$ indeed generally depends on $x_{\|}$. We therefore conjecture that the above behaviors of $x_{\rm app}$ for $x_{\|} < 1$ and $x_{\|} > 1$ hold for other models as well. It is interesting to note that this is exactly the same criterion for ϕ being relevant or irrelevant at the surface, respectively. For the case without a crossover ($\langle\phi\rangle \neq 0$), one has in general $x_{\|} = 2$.[12]

As for applications, another important boundary condition is obtained by applying a random field coupling to the order parameter at the boundary.[13,14] For a two-dimensional adsorption system one can argue that irregularities of the boundary on scales of a few lattice sites can be modeled this way. Due to an uneven edge, some boundary sites may be more probable than others, corresponding to a local boundary field favoring those sites. Such a random boundary field is irrelevant for $x_{\|} > \frac{1}{2}$, with $x_{\|}$ the surface exponent of the order parameter for a free boundary.[14] Thus we expect free-boundary predictions to apply in this case. However, for $x_{\|} \leq \frac{1}{2}$ one has to carry out a more detailed analysis.

MULTICRITICAL ISING MODELS

In order to test the predictions for $x_{\rm app}$, we have computed a number of apparent scaling relations at the $\mathbb{Z}_2$-invariant N-critical point of a φ^{2N}-Landau-Ginzburg theory. These so-called N-critical Ising models can be mapped to the unitary series of minimal models $\mathcal{M}_m$, $m = N + 1 = 3, 4, \ldots$ in conformal field theory,[15] which have also been identified by Huse[16] with certain multicritical transitions in the restricted solid-on-solid (RSOS) models — solved exactly by Andrews, Baxter, and Forrester in a two-dimensional subspace of the full parameter space.[17]

With $\mathcal{M}_m$ viewed as a ferromagnetic model, the order parameter φ is the magnetization σ and identified with the most relevant primary operator. The second relevant operator (energy density ϵ) is given by the renormalized composite field $:\!\varphi^2\!:$ defined as the leading operator in the OPE-expansion of $\varphi\varphi - \langle\varphi\varphi\rangle$. Higher operators are similarly classified as spinlike or energylike, which are $\mathbb{Z}_2$ odd or even, respectively, under spin reversal ($\sigma \to -\sigma$).

Our calculations have been performed for a disk with fixed or free boundary conditions. The structure factor in (1), reduced to a three-dimensional integral due to the rotational symmetry of the disk, has been evaluated numerically using Gaussian quadratures and a mesh of 60^3 points or more. The exact spin-spin correlation functions $\langle\sigma\sigma\rangle_c$ for restricted domains[18] provide a range of candidates for this test. The results for the bi-, tri-, and tetracritical Ising models with fixed and free boundary conditions are given in Fig. 2. To provide an example of an energylike operator, we have carried out the corresponding analysis for the tricritical energy density ϵ as well. The results for fixed and free boundary conditions are identical and look essentially like those for the order parameters in Fig. 2 for fixed boundary conditions. (The exact curve is given in Fig. 7 in Ref. 3.)

These exact calculations all confirm the predictions summarized in Fig. 1. For the spin operators, we have for fixed boundary conditions $\langle\sigma\rangle \neq 0$ and $x_{\|} = 2$, and for free boundary conditions $\langle\sigma\rangle = 0$ and

$$x_{\|} = \begin{cases} 1 + \frac{2}{m}, & m \text{ even}, \\ 1 - \frac{2}{m+1}, & m \text{ odd}, \end{cases} \tag{12}$$

for $m = 3, 4, \ldots$.[18] The condition $\bar{x}' < 1$ follows from $x' \leq 1$ for all models. For the tricritical energy density, $\langle\epsilon\rangle \neq 0$ for both fixed and free boundary conditions and the surface exponent $x_{\|} = 2$ in both cases. However, as $x' = \frac{6}{5}$, it is not *a priori* clear whether the average exponent $\bar{x}' < 1$. But, as we know the exact result, we

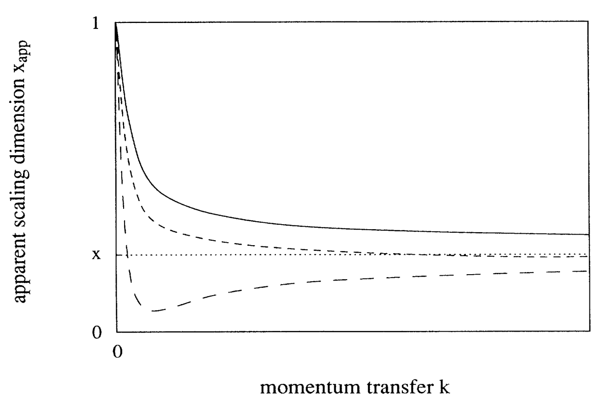

FIG. 1. Generic apparent scaling dimensions $x_{\rm app}$ vs momentum transfer k. The solid line corresponds to $\langle\phi\rangle \neq 0$ ($x_{\|} = 2$), while the lower curves illustrate $\langle\phi\rangle = 0$. For the short (long)-dashed curve $x_{\|} > 1$ (< 1). The dotted line shows the bulk scaling dimension x to which $x_{\rm app}$ converges.

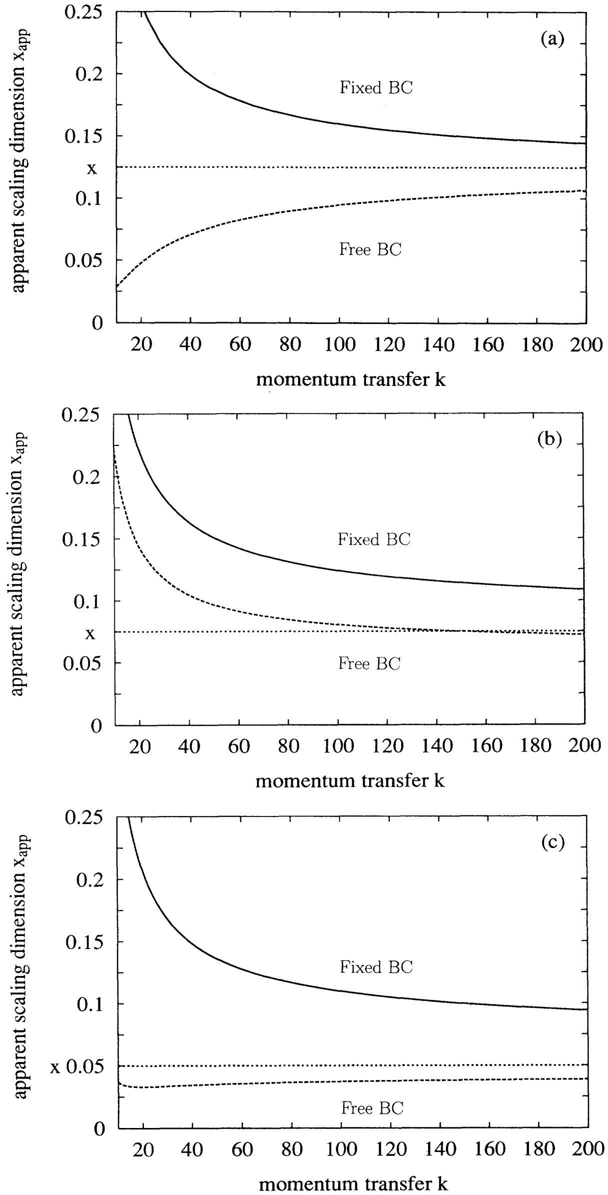

FIG. 2. Apparent scaling dimensions $x_{\rm app}$ vs momentum transfer k, starting at $k = 10$, for the order parameters σ of the (a) bi-, (b) tri-, and (c) tetracritical Ising models in a disk of unit radius. For fixed boundary conditions ($\langle\sigma\rangle \neq 0$), the surface exponents $x_\parallel = 2$, whereas for free boundary conditions ($\langle\sigma\rangle = 0$), $x_\parallel = \frac{1}{2}$, $\frac{3}{2}$, and $\frac{2}{3}$, respectively. The corresponding scaling dimensions are $x = \frac{1}{8}$, $\frac{3}{40}$, and $\frac{1}{20}$, shown with dotted lines.

can conclude that this must be the case, because we get $x_{\rm app} < x$ at large k for $\bar{x}' > 1$.

We conclude from (12) that the random boundary field is irrelevant for all multicritical Ising models except the bicritical one, for which it is marginal[14,19] ($x_\parallel = \frac{1}{2}$). In this case Cardy has shown that it leads to an order-parameter profile corresponding to that of a fixed boundary.[14] This suggests that the fixed-boundary prediction applies in this case.

SUMMARY

We have shown how the apparent power law of a structure factor in a bounded two-dimensional domain at a critical point depends on the boundary conditions. Whether the scaling dimensions are over- or underestimated can be predicted from simple symmetry analyses or the corresponding surface exponents.

To be able to compare the predictions and the calculations presented in Figs. 1 and 2 with a physical system or a lattice model, one has to set a proper length scale. By multiplying all lengths by R^{-1}, with $2R$ the characteristic length of a system, a comparison with the unit-radius disk can be made, as the line shape of the structure factor is invariant under such a scale transformation if one simultaneously rescales the momenta by R. One must also keep in mind that the calculations have been carried out in the continuum limit, i.e., that there is an upper bound for the momenta of the order of an inverse lattice constant a^{-1}. For a system with $2R/a = 100$ sites per length dimension, for example, this corresponds to a normalized momentum $k < 50$. Hence, the effects of apparent scaling as predicted and computed here indeed cover the significant range of momenta. Moreover, the effects are even more pronounced at lower momenta, where accuracy is higher for both experimental measurements and numerical calculations.

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* Electronic address: tfkpf@fy.chalmers.se

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