CORRECTIONS TO SCALING AND FINITE SIZE EFFECTS

H.J. HERMANN

Service de Physique Théorique, CEN Saclay, 91 191 Gif sur Yvette Cédex, France

and

D. STAUFFER

Institut für Theoretische Physik, Universität zu Köln, Zülpicherstr. 77, 5000 Cologne 41, West Germany

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Numerical investigations of critical phenomena might lead to different leading correction-to-scaling terms, depending on the type of analysis. We discuss which leading correction-to-scaling behavior is expected for finite system sizes, using two-dimensional percolation as our main example. It turns out that a finite-size scaling from length $L$ to $L - 1$ is less perturbed by correction-to-scaling terms.

Any accurate analysis of experimental or numerical data in terms of critical properties near second-order phase transition has to take into account that scaling laws and critical exponents etc. are defined asymptotically close to the critical point. At any finite distance from the critical point one has to take into account additional corrections to scaling terms, which influence the analysis for the leading nonanalyticity, even though their relative importance vanishes right at the critical point.

Recently Privman and Fisher [1] discussed the effect of corrections to scaling in numerical methods with finite-size effects and they illustrated their results with some series expansions. Although we agree with their conclusion that a renormalization of finite strips of width $L$ to width $L - 1$ has a specially weak correction to finite size scaling, we cannot follow their argument that there is a spurious cancellation for $L \leq 10$ in the case of percolation [2]. We discuss the corrections to finite-size scaling that arise if one does not compare systems of sizes $L$ and $L - 1$.

Two main sources for corrections to scaling are believed to exist in the bulk: one is the influence of irrelevant scaling fields $g_{T}$ [3] which yields exponents $\Delta_{T}$ that are not related to the usual critical exponents like $\gamma_{T}$ and $\gamma_{H}$. For simplicity we allow for only one such irrelevant field, which is the one with the smallest exponent $\Delta_{T}$. Then the free energy $F$ per unit volume has the form

$$F = g_{T}^{d/\gamma_{T}} f_{1}(g_{T}^{-\Delta_{T}}, g_{H}^{\gamma_{H}/\gamma_{T}}) + g_{T}^{-\Delta_{T} + d/\gamma_{T}} f_{1}(g_{T}^{-\Delta_{T}}, g_{H}^{\gamma_{H}/\gamma_{T}}) + \ldots,$$

where $f$ and $f_{1}$ are scaling functions and $g_{T}, g_{H}$ are the relevant scaling fields related to $T - T_{c}$ and "magnetic field" $H$; the exponents $d/\gamma_{T}$ may be written as $d \nu + 1 - \alpha$ in $d$ dimensions, and the ratio $\gamma_{H}/\gamma_{T}$ as $\beta_{5} / \beta + \gamma$.

The other source of correction terms is the (nonlinear) mixture of the scaling fields, as pointed out recently by Aharony and Fisher [4]. That means that the scaling fields can be approximated close to the critical point by Taylor expansions:

$$g_{T} = T - T_{c} + a_{1} H + a_{2} (T - T_{c})^{2} + a_{3} H^{2} + a_{4} (T - T_{c}) H + \ldots,$$

$$g_{H} = H + b_{1} H^{2} + b_{2} (T - T_{c}) H + \ldots.$$  

In models with an exact symmetry between positive and negative fields $H$, some of these terms vanish.
This effect produces also correction terms to the leading free energy, but the exponents can be expressed in terms of the normal exponents $\gamma_H$ and $\gamma_T$. We now assume \[ a_1 \neq 0 \] for percolation.

For example in the model with no symmetry between $H$ and $-H$ has at $T = T_c$ \[ F = H^{d_H}y_H(A + BH^{1-\gamma_T/\gamma_H} + CH^{\Delta_1 \gamma_T/\gamma_H} + ...) \]. \hspace{1cm} (3)

Thus if the "irrelevant" exponent $\Delta_1$ is larger than $\gamma_H/\gamma_T - 1$, then the leading correction terms $H^{d_H \gamma_T/\gamma_H}$ is given by the usual exponents whereas in the opposite case the leading correction term $H^{\Delta_1 \gamma_T/\gamma_H}$ comes from the irrelevant field.

In the case of percolation \[ s = 1/H \] is the number of sites in a cluster. For two dimensions, $1 - \gamma_T/\gamma_H = 1 - \alpha = 55/91 = 0.6$ is smaller than $\Delta_1 \gamma_T/\gamma_H = \Delta_1 \times 36/91 = (\gamma_2/\gamma_T) \times 36/91 = 96/91 = 1.05$, when $\gamma_2 = 2$ is used \[ 7 \] for the leading irrelevant field, and $\gamma_T = 3/4$. Thus the leading correction to scaling comes from eq. (2) and not from the irrelevant field, in agreement with the numerical analysis of cluster number right at the critical point \[ 5 \].

We now apply these known concepts to finite-size scaling. Many numerical methods do not obtain critical exponents by varying the fields $g_T$ or $g_H$ but instead by varying the system size right at the critical point $g_T = g_H = 0$. Although scaling laws can be formulated involving the system linear dimension $L$ in a way completely analogous to $g_T$ and $g_H$ \[ 8 \], in the renormalization group sense ref. \[ 9 \] does not treat the size $L$ as a scaling field. Thus $L$ will not change eq. (2) and no new irrelevant operators arise from the finite system size. Therefore we take the free energy in an large but finite system as

\[ F = g_T^{d_H \gamma_T} f(x, y, z) + g_T^{\Delta_1 + d_H \gamma_T} f_1(x, y, z) + ..., \] \hspace{1cm} (4)

with the abbreviations $x = g_T^{d_H \gamma_T}, y = g_T^{\gamma_T/\gamma_H}T$ and $z = g_T^{\gamma_T}$. For finite systems any phase transition is smeared out, and thus the free energy should be analytic if the critical point is reached, $g_T = g_H = 0$, in a finite system, $L < \infty$. Therefore the scaling functions $f(x, y, z)$ and $f_1(x, y, z)$ behave asymptotically in such a way that the corresponding terms in eq. (4) are proportional to some powers of $L$ at the critical point. Now eq. (4) gives, for $g_T = g_H = 0$, i.e. if one studies the system exactly at the bulk critical point:

\[ F = L^{-d} (\tilde{A} + \tilde{B} L^{-\omega} + ...), \] \hspace{1cm} (5)

where $\omega = \Delta_1 \gamma_T = \gamma_2$ in the notation of ref. \[ 7 \]. If $\gamma_2 = 2$ for two-dimensional percolation, the correction term of eq. (5) will be weak.

Very often, however, the critical point is not known exactly and a numerical approximation $g_T^c(L)$ of the critical point $g_T^c = 0$ is calculated where $g_T^c(L) \to 0$ for $L \to \infty$. Then an additional correction to eq. (5) due to the deviation from the exact critical point arises and one gets

\[ F = L^{-d} (\tilde{A} + \tilde{B} L^{-\omega} + \tilde{C} g_T^c(L) L^{\gamma_T L} + ...). \] \hspace{1cm} (6)

The way how $g_T^c(L)$ decreases for large $L$ strongly depends on the numerical method used to calculate $g_T^c(L)$ and the corrections to scaling in (6) will vary very much with the numerical method. These corrections at the end determined the convergence of a numerical method.

In the following we will therefore discuss the $L$ dependence of $g_T^c(L)$ for some numerical methods.

We assume that we determine a size dependent critical point $T_c(L)$ or $g_T^c(L)$ by the requirement that the specific heat $C_V$ (or the susceptibility) has a maximum there. We assume

\[ (dC_V/dT) L = \varphi((g_T + \alpha g_T^2 + ...) L^{\gamma_T L}) + ... \] \hspace{1cm} (7)

The maximum is found by setting this derivative equal to zero, giving $L^{\gamma_T L} g_T^c(L)[1 + O(g_T^c(L))] = \text{constant}$ and thus

\[ g_T^c \alpha L^{\gamma_T L} \] \hspace{1cm} (8)

and analogously for $T_c(L) - T_c(\infty)$. Combined with the previously discussed $L^{-\omega}$ correction we obtain

\[ g_T^c(L) = L^{\gamma_T L} (a + b L^{-\omega} + c L^{\gamma_T L} + ...). \] \hspace{1cm} (9)

The leading term $L^{\gamma_T L}$ is well known \[ 10 \]. The correction term in $L^{-\omega}$ makes no qualitative change compared to eq. (5) (except in the improbable situation $\tilde{B} = -b \tilde{C}$). The correction term in $L^{\gamma_T L}$ gives an additional correction to eq. (5) and if $\gamma_T < \omega$ as for instance in two-dimensional percolation ($\gamma_T = 3/4$, $\omega = 2$) the convergence to $L \to \infty$ is much better for a method at the exact critical point $g_T = 0$ as in eq. (5) than for a method where the critical point is determined from the maximum (or the inflection point etc...) of a given quantity. Of course further corrections terms in eq. (9) arising from other reasons are also possible.
A method which is sometimes used to obtain \( g_T^L(L) \) in geometrical problems is to calculate the probability \( R_L(p) \) to percolate through a \( L \times L \) cell with a site or bond probability \( p \) and to define the \( L \)-dependent threshold \( g_T^L(L) = (p_L - p_c) + \ldots \) by \[ R_L(p_L) = p_L, \] (10)
or \[ p_L = \frac{1}{\rho} \int p(d\rho/dp)dp, \] (11)

and where \( p_c \) is or exactly known \[ 12 \] or extrapolated from \( g_T^L(L) \to 0 \) for \( L \to \infty \) \[ 11 \]. For both cases finite size scaling yields a behavior of the type of eq. (9) so that a correction term \( L^{-\gamma_T} \) is present. As already mentioned this term will dominate the correction to scaling behavior in the case of two dimensional percolation. Indeed the value 0.65 to 0.85 \[ 13 \] estimated for the leading correction exponent from the correlation length calculated in ref. \[ 12 \] is compatible with \( \gamma_T \approx 3/4 \). For other ways to extract the correction to scaling exponents see ref. \[ 14 \].

Another method to obtain \( g_T^L(L) \) is a finite-size renormalization with system of lengths \( L \) and \( L - 1 \) \[ 15 \] for instance by using for the correlation length \( \xi_L \) is a system with a length \( L \) an equation \[ (L - 1)\xi_L(g_T^L) = L\xi_{L-1}(g_T^L). \] (12)

Applying finite size scaling one obtains in this case \[ 1,2 \]:

\[ g_T^L(L) = L^{-\gamma_T}(bL^{-\omega} + dL^{-2\omega} + \ldots). \] (13)

We see that the leading shift varies as \( L^{-\gamma_T-\omega} \), no \( L^{-\gamma_T} \) correction appears in this case and for \( \gamma_T < \omega \) this method has a better convergence than the other methods presented before. This is presumably the reason why methods of this type usually give good results already for small \( L \) \[ 15 \]. That the leading correction exponent is in this case indeed \( \omega \) is seen for two dimensional percolation from the calculations on strips of Derrida and de Seze who found an exponent of the order of two agreeing with the result \( \omega = 2 \) of ref. \[ 7 \]. So their value is not due to a spurious cancellation as asserted in ref. \[ 1 \] but agrees well with the expected value.

To check this result, we show in fig. 1 a somewhat more systematic attempt to extract the correction exponent \( \omega \) from the data of Derrida and de Seze, similar to the analysis employed in ref. \[ 5 \]. From consecutive values for \( L \) the effective correction exponent of eq. (5) was determined from the values of \( 1/\gamma_T \) [and similarly also from the values for \( p_c(L) \)] tabulated by Derrida and de Seze. We see in the various examples that the data first increase with increasing \( L \) and seem to approach a limit above 2 for \( \omega \); but in the last point a downward curvature is clearly visible, making an extrapolation of \( \omega \) to 2 for infinite \( L \) not un plausible. Much longer series would be needed to show \( \omega = 2 \) convincingly.

In all the reasoning up to now we have considered the behavior of convergence in the large \( L \) limit. In practical calculations, however, the amplitudes \( A, B, C \) in eq. (6) or \( a, b, c \), in eq. (9) play an important role in the range of not too large \( L \). The amplitudes which vary from method to method will together with the leading correction exponents ultimately decide which numerical method is the most appropriate for a given problem. If one could find a method in which for instance the \( b \) of eq. (13) fulfills \( b = -B/C \) in eq. (6) the
leading correction exponent would be 4 at two-dimensional percolation thresholds.

In summary we have seen that if the critical point is not exactly known the method of renormalizing from a length \( L \) to \( L - 1 \) has a special cancellation of terms in the finite-size scaling which can give numerically much better results if \( \omega > \nu_T \). This is the case for two-dimensional percolation where we have reanalyzed different numerical methods and found that the correction to scaling exponents of the different methods are consistent with our picture. However, our theory is based on several assumptions \([4,5,7,9]\) which at present are unproven. To distinguish numerically between the predictions of Privman and Fisher \([1]\) and our alternative much better computer data seem needed.

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References