Finite-size analysis of first-order phase transitions: Discrete and continuous symmetries

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First-order phase transitions are characterized by δ-function singularities in thermodynamic quantities. The way in which these singularities develop in taking the thermodynamic limit is qualitatively different for finite systems and systems infinite in one direction only. The corresponding crossover behavior, which we predict in detail with a renormalization-group analysis, is a unique feature of first-order transitions and is suggested to be of considerable utility. Both systems with discrete and continuous symmetries are discussed. For the latter we verify our results for the two geometries within the spin-wave approximation.

I. INTRODUCTION

A wealth of information about critical behavior of infinite systems can be derived from a study of their finite counterparts. Research in recent years has most vividly borne this out. Both finite-size scaling and phenomenological renormalization have been very successful in this respect.[1–4]

The usual, physically appealing, argument on which finite-size scaling relies invokes the scale invariance of a system with an infinite correlation length, i.e., a critical system.[5] In the critical region the properties of the system depend only on the ratio of the finite size and the correlation length: the dimensionless combination of the only two physically relevant length scales. For a system with a first-order transition the correlation length remains finite and the scale invariance is lost. So is finite-size scaling, along this line of reasoning.

Alternatively, finite-size scaling can be considered to be an application of renormalization-group theory.[6] The essence of this formulation is as follows: (1) The renormalization-group equations are those of the infinite system; and (2) an additional relevant scaling field, viz., the inverse linear dimension, is responsible for the finite-size behavior (the corresponding scaling index equals one). These two assumptions account for the dominant finite-size singularities.

The renormalization-group formulation of finite-size scaling is the more general and powerful one. For example, it immediately yields Suzuki's extension of finite-size scaling to critical dynamics.[7] Not unusual for first-order transitions, it has recently been suggested that also finite-size scaling for first-order transitions can be understood in terms of a zero-temperature, discontinuity fixed point.[6,8,9]

The purpose of this paper is twofold. First, we want to stress that the unique finite-size signature of a first-order transition is the qualitatively distinct behavior of finite systems and systems infinite in one direction only. Since the latter are intractable, e.g., in simulations, we consider in detail the crossover between the two geometries and the corresponding data collapse. The analysis of first-order transitions suggested—where finite-size dependence is exploited rather than carefully avoided—is definitely more elegant. Moreover, it may very well be more powerful, as indeed it is in the case of continuous transitions.

Second, we present a calculation that corroborates the conclusion based on the discontinuity fixed-point analysis. This suggests that the renormalization arguments, crude as they might be, apparently capture the correct physics.

II. SCALING THE HYPERCUBIC PRISM

We consider a finite system on a d-dimensional hypercubic lattice: a hypercubic prism with periodic boundary conditions. The prism has linear size n in $d-1$ dimensions and m in the remaining dimension.

For definiteness take a p-component Heisenberg model with reduced Hamiltonian (i.e., a factor $-k_BT$ is included):

$$\mathscr{H}=K\sum_{(i,j)}\vec{s}_i\cdot\vec{s}_j+h\sum_i s_i^1\ , \tag{1}$$

where (i,j) runs through all nearest-neighbor sites and $\vec{s}_i=(s_i^1,\ldots,s_i^p)$ is a p-dimensional unit vector.

For $K > K_c$ the system spontaneously orders, say, along the $(1,0,\ldots,0)$ direction. Equivalently, the corresponding susceptibility has a δ function concentrated at $h=0$. In a finite system the δ function will be approximated by a smooth peak of ever increasing height as the system tends to the thermodynamic limit. We are interested in this height as a function of system size.

Sufficiently close to the discontinuity fixed point the renormalization equations, corresponding to a length rescaling factor L, are

$$T' = L^{-y}T, \quad h' = L^{d}h , \tag{2}$$

where $T = K^{-1}$ and

$$y = \begin{cases} d-1 & \text{for } p=1 , \\ d-2 & \text{for } p>1 \text{ and } d>2 . \end{cases} \tag{3}$$

Note that y differs for systems with a discrete[10] or continuous[11] symmetry. The free energy in units $k_B T$ per site f satisfies

$$f(T,h,n^{-1},m^{-1}) = L^{-d} f(L^{-y}T, L^{d}h, Ln^{-1}, Lm^{-1}) . \tag{4}$$

Note that a background term in the free energy was ignored. The exponent d associated with h is the discontinuity exponent[12] which gives rise to a nonzero order parameter. Equation (4) implies that the susceptibility $\chi = \partial^2 f/\partial h^2$ in zero field satisfies

$$\chi(T,n^{-1},m^{-1}) = L^{d}\chi(L^{-y}T, Ln^{-1}, Lm^{-1}) . \tag{5}$$

With the choice $L=n$ one obtains

$$\chi(T,n^{-1},m^{-1}) = n^{d}\chi(n^{-y}T, 1, n/m) , \tag{6}$$

which expresses the susceptibility of a d-dimensional system of $n^{d-1}m$ sites in terms of that of a one-dimensional chain of length $l = m/n$. If we now parametrize the latter in terms of its inverse correlation length κ rather than T, we find (see the Appendix)

$$\chi(\kappa, l^{-1}) = l\hat{\chi}(l\kappa) , \tag{7}$$

with

$$\hat{\chi}(x) \sim \begin{cases} 1 & \text{for } x \ll 1 , \\ 2/x & \text{for } x \gg 1 . \end{cases} \tag{8}$$

Since

$$\kappa = \begin{cases} e^{-2K} & \text{for } p=1 \quad (K \gg 1) , \\ \frac{1}{2}(p-1)T & \text{for } p>1 , \end{cases} \tag{9}$$

it then follows that

$$\chi(T,n^{-1},m^{-1}) = \begin{cases} n^{d-1}m\hat{\chi}\left[\dfrac{m}{n}\exp(-2n^{d-1}K)\right] \\ n^{d-1}m\hat{\chi}\left[\dfrac{m(p-1)}{2n^{d-1}K}\right] . \end{cases} \tag{10}$$

This is our main result: $\chi/n^{d-1}m$ depends only on a combination of the two parameters m and n. The scaling functions $\hat{\chi}$ as obtained within our approximation are given in the Appendix. Note that from Eqs. (10) one immediately recovers the previously reported results

$$\chi \sim n^{d} \tag{11a}$$

for a system of $n \times \cdots \times n$ sites, and

$$\chi \sim \begin{cases} n^{d}\exp(2n^{d-1}K) & \text{for } p=1 \\ n^{2d-2} & \text{for } p>2 \end{cases} \tag{11b}$$

for the semi-infinite case of $\infty \times n \times \cdots \times n$ sites.[2,6]

It is illuminating to contrast the behavior for a first-order transition [Eqs. (10)] with the corresponding result for a continuous transition. Using arguments similar to those employed above in the latter case one obtains

$$\chi(T_c,n^{-1},m^{-1}) \simeq n^{2y_h-d}\chi(T_c,1,n/m) = n^{2y_h-d}\left[A + B\exp\left[-\frac{m\kappa}{n}\right]\right] , \tag{12}$$

where y_h is the magnetic critical exponent and A, B, and κ may be obtained by calculating a one-dimensional susceptibility. Comparing Eqs. (10) and (11) one sees that the difference between first-order and continuous transitions in the $m \simeq n$ region may be arbitrarily small if $y_h \lesssim d$. However, a clear distinction is always found in principle for $m \gg n$.

In the derivation above we have assumed that T is sufficiently small that the renormalization equations (2) hold. To extend the validity of the analysis one replaces T and h by the appropriate scaling fields. The only implication is that K in Eqs. (10) and (11) becomes an unknown constant. Equations (10) and (11) are also expected to apply to the peak in the specific heat for a system with a latent heat. In a renormalization-group context the temperature deviation from the transition couples to an ordering field at the discontinuity fixed point and thus plays the role of h above.[13] We caution the reader that in a system with a continuous symmetry the latent heat may very well be associated with a $T=0$ coexistence of phases separated by a finite energy gap. In that case the $p=1$ analysis applies.

III. FINITE-SIZE BEHAVIOR: THE SPIN-WAVE APPROXIMATION

As in the preceding section we consider here the p-component Heisenberg model on a hypercubic lattice. We shall establish the finite-size behavior as predicted by the renormalization-group analysis for the $n\times\cdots\times n$ and $\infty\times n\times\cdots\times n$ geometries [cf. Eqs. (11)]. For this purpose a spin-wave approximation is employed.

At low temperatures, and for $d>2$, the spin-spin correlation function can be approximated by[14]

$$\langle\vec{s}(\vec{r})\cdot\vec{s}(\vec{0})\rangle\sim\exp\{(p-1)[G(\vec{r})-G(\vec{0})]\}, \tag{13}$$

with $\vec{r}=(r_1,\ldots,r_d)$ and $\vec{0}=(0,\ldots,0)$ labeling lattice sites. For the infinite system

$$G(\vec{r})=G_\infty(\vec{r})=\frac{1}{2K}\int\frac{d\vec{k}}{(2\pi)^d}\frac{e^{i\vec{k}\cdot\vec{r}}}{\sum_{i=1}^{d}(2-2\cos k_i)}, \tag{14}$$

the integral being over the first Brillouin zone: $|k_i|\le\pi$. For finite systems or systems infinite in one direction only, the integral above has to be modified appropriately, as discussed in detail below. For an infinite system or a finite system with periodic boundary conditions the susceptibility is given by

$$\chi=\sum_{\vec{r}}\langle\vec{s}(\vec{r})\cdot\vec{s}(\vec{0})\rangle\ . \tag{15}$$

We now treat the following two geometries.

Case 1: A hypercube of length n all d dimensions

The pertinent Green's function, denoted by $G_n(\vec{r})$, is obtained from Eq. (14), making the substitution

$$\int\frac{d\vec{k}}{(2\pi)^d}\to\frac{1}{n^d}\sum_{\vec{k}\neq\vec{0}}, \tag{16}$$

where the sum is over $k_i=0,\pm2\pi/n,\ldots$. The following inequality holds:

$$0\le G_n(\vec{r})\le G_n(\vec{0})\ . \tag{17}$$

The right-hand side of this relation is obvious. The physics contained in the left-hand side is also clear: G_n is the correlation function of ferromagnetically coupled Gaussian variables. To prove this side of the inequality exactly, one applies a theorem by Stieltjes and Ostrowski[15]: $G_n\ge0$ being the inverse of a positive-definite matrix—the eigenvalues are $\sum_{i=1}^{d}(2-2\cos k_i)$, $\vec{k}\neq\vec{0}$—with positive diagonal and nonpositive off-diagonal elements (proportional to 2 and -1 or 0, respectively). For the susceptibility χ_n one obtains

$$\sum_{\vec{r}}\exp[-(p-1)G_n(\vec{0})]\le\chi_n\le\sum_{\vec{r}}1\ . \tag{18}$$

As $n\to\infty$ one has $G_n(\vec{0})\to G_\infty(\vec{0})$, which is finite. Therefore, a constant c, independent of n, exists such that

$$\exp[-(p-1)G_n(0)]>c>0\ .$$

It then immediately follows that

$$\chi_n\sim n^d \text{ as } n\to\infty\ ,$$

which verifies Eq. (11a).

Case 2: A system infinite in one dimension and of linear size n in $d-1$ dimensions

Assume the system to be infinite along the 1 direction. One now replaces in Eq. (14)

$$\int\frac{d\vec{k}}{(2\pi)^d}$$

by

$$\frac{1}{n^{d-1}}\sum_{\vec{k}_\perp}\int\frac{dk_1}{2\pi}, \tag{19}$$

where $k_{\perp i}=0,\ \pm2\pi/n,\ldots$. Denote by $\tilde{G}_n$ the Green's function obtained in this way. Note that, as opposed to (16), the term $\vec{k}_\perp=\vec{0}$ is included in the sum. Treating this term separately we write

$$\tilde{G}_n(\vec{r})-\tilde{G}_n(\vec{0})=\tilde{G}'_n(\vec{r})-\tilde{G}'_n(\vec{0})+F(z)/n^{d-1}, \tag{20}$$

where

$$\tilde{G}'_n(\vec{r})=\frac{1}{2Kn^{d-1}}\sum_{\vec{k}_\perp\neq0}\int\frac{dk_1}{2\pi}\frac{e^{i\vec{k}\cdot\vec{r}}}{\sum_{i=1}^{d}(2-2\cos k_i)} \tag{21}$$

and

$$F(z)=\frac{1}{2K}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\frac{e^{ikz}-1}{2-2\cos k}=-\frac{1}{4K}|z|\ . \tag{22}$$

Taking the appropriate limit in the inequality (17) one obtains

$$0\le\tilde{G}'_n(\vec{r})\le\tilde{G}'_n(\vec{0}), \tag{23}$$

noting that the $\vec{k}_\perp=0$ terms in Eq. (21) give rise to corrections of order n^{1-d} in the nonzero elements of the inverse of $\tilde{G}'_n$, so that the Stieltjes-Ostrowski theorem still applies. Hence the susceptibility $\tilde{\chi}_n$ satisfies

$$\exp[-(p-1)\tilde{G}'_n(0)]\sum_{\vec{r}}\exp\left[-\frac{p-1}{4Kn^{d-1}}|z|\right]\leq\chi_n\leq\sum_{\vec{r}}\exp\left[-\frac{p-1}{4Kn^{d-1}}|z|\right]. \quad (24)$$

Once again $G'_n(\vec{0})\to G_\infty(\vec{0})$ as $n\to\infty$, so that $\exp[G'_n(0)]>c$ for positive constant c independent of n. Furthermore,

$$\sum_{\vec{r}}\exp\left[-\frac{p-1}{4Kn^{d-1}}|z|\right]\simeq 4n^{2d-2}K/(p-1) \quad (25)$$

and

$$\chi_n\sim\frac{K}{p-1}n^{2d-2}.$$

This, then, establishes our result in (11b).

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APPENDIX

We derive Eqs. (8) and (9) and calculate the scaling function $\hat{\chi}$. As a by-product the integral in Eq. (22) is evaluated.

Consider a chain of spins $\vec{s}_0,\vec{s}_1,\ldots,\vec{s}_{l-1}$ with periodic boundary conditions: $\vec{s}_l\equiv\vec{s}_0$. For $p=1$ (Ising chain) the correlation function is

$$\langle s_0s_r\rangle=\frac{\exp(-\kappa r)+\exp[-\kappa(l-r)]}{1+\exp(-\kappa l)}, \quad (A1)$$

with the inverse correlation length given by $\kappa=-\ln\tanh K\simeq e^{-2K}$ for large K. By summing over r one obtains the susceptibility, and for low temperatures

$$\chi(\kappa,l^{-1})\simeq l\hat{\chi}(l\kappa), \quad (A2)$$

with

$$\hat{\chi}(x)=\frac{2(1-e^{-x})}{x(1+e^{-x})}. \quad (A3)$$

The function $\hat{\chi}$ indeed satisfies Eq. (8).

For $p>1$ the correlation function in the spin-wave approximation is

$$\langle\vec{s}_0\cdot\vec{s}_r\rangle\sim\left[\frac{\mathrm{Tr}\exp\left[i\phi_r-K\sum_{j=0}^{l-1}(\phi_{j+1}-\phi_j)^2\right]}{\mathrm{Tr}\exp\left[-K\sum_{j=0}^{l-1}(\phi_{j+1}-\phi_j)^2\right]}\right]^{p-1}, \quad (A4)$$

where

$$Tr=\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}d\phi_1\cdots d\phi_{l-1}.$$

Now introduce a transfer matrix,

$$T(\phi,\psi;K)=\sqrt{K}\exp\left[-\frac{K}{2}(\phi-\psi)^2\right]. \quad (A5)$$

The eigenvalues and eigenvectors are $\exp(-k^2/2K)$ and $[\exp(ik\phi)]/\sqrt{2\pi}$. It then immediately follows that the transfer matrix to the power m satisfies

$$T^m(\phi,\psi;K)=T(\phi,\psi;K/m) \quad (A6)$$

for any positive m. The correlation function (A4) can then be written as

$$\langle\vec{s}_0\cdot\vec{s}_r\rangle\sim\left[\left[\frac{l}{K}\right]^{1/2}\int_{-\infty}^{\infty}d\phi_r T\left[\phi_0,\phi_r;\frac{K}{r}\right]\exp(i\phi_r)T\left[\phi_r,\phi_0;\frac{K}{l-r}\right]\right]^{p-1}$$
$$\sim\exp\left[-(p-1)\frac{r(l-r)}{4Kl}\right]. \quad (A7)$$

The inverse correlation length is

$$\kappa=(p-1)/4K.$$

For large l the susceptibility can readily be obtained and reads

$$\chi(\kappa,l^{-1})=l\hat{\chi}(l\kappa),$$

with

$$\hat{\chi}(x)=\int_0^1\exp[-y(1-y)x]dy, \quad (A8)$$

which again satisfies Eq. (8). Equations (14) for $d=1$ and (A7) for $l\to\infty$ immediately give Eq. (22).

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