Order-Parameter Distribution Function of Finite $O(n)$ Symmetric Systems

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(Received 2 April 1996)

We present analytic and numerical studies of the order-parameter distribution function near the critical point of $O(n)$ symmetric three-dimensional (3D) systems in a finite geometry. The distribution function is calculated within the φ^4 field theory for a 3D cube with periodic boundary conditions by means of a new approach that appropriately deals with the Goldstone modes below T_c. Good agreement is found with new Monte Carlo data for the distribution function of the magnetization of the 3D *XY* ($n = 2$) and Heisenberg ($n = 3$) models. [S0031-9007(96)01500-1]

PACS numbers: 75.40.Mg, 05.70.Jk, 64.60.Ak

The interest in analytic and numerical studies of finite-size effects on phase transitions has remained on a highly stimulating level over the last years. Perhaps the most fundamental quantity in the statistical description of these effects is the probability distribution $P(\Phi)$ of the spatial average Φ of the order parameter [1], $\Phi = V^{-1}\int d^dx\,\varphi(x)$ or $\Phi = N^{-d}\sum_i \varphi_i$, where $\varphi(x)$ and φ_i represent the local fluctuating order-parameter variable in a continuum or discrete description with V and N^d being the finite volume or number of lattice sites, respectively. This distribution function can be studied analytically and numerically both for Ising-like systems as well as for $O(n)$ symmetric systems (such as *XY* and Heisenberg models) where Φ is an n component vector. The latter systems are of particular interest below T_c because of the massless spin-wave (Goldstone) modes governing the long-distance properties.

While detailed numerical studies on $P(\Phi)$ have been carried out for the three-dimensional (3D) Ising model [1,2], no numerical results are available (to the best of our knowledge) for $O(n)$ symmetric 3D systems with $n > 1$. This corresponds to the situation on the theoretical side where no predictions are available for the critical behavior of $P(\Phi)$ in finite 3D systems with an n-component order parameter with $n > 1$. This lack of theoretical knowledge is related to the notorious difficulty in treating the Goldstone modes near criticality. In fact, so far the existing field-theoretic approaches to finite-size effects within the φ^4 model [3–7] are not appropriate to satisfactorily deal with the Goldstone problems related to $P(\Phi)$ for $T \lesssim T_c$. The goal of this Letter is to fill in this gap. We shall calculate $P(\Phi)$ for general n above and below T_c on the basis of a novel finite-size approach and shall compare the resulting finite-size scaling function with new Monte Carlo (MC) data of the 3D *XY* and Heisenberg models. Good agreement between the MC data and the theoretical predictions is found.

Our analytic treatment is based on the φ^4 model with the standard Landau-Ginzburg-Wilson Hamiltonian

$$H = \int_V d^dx\left[\tfrac{1}{2}r_0\varphi^2 + \tfrac{1}{2}(\nabla\varphi)^2 + u_0\varphi^4\right], \qquad (1)$$

where $\varphi(x) = L^{-d}\sum_k \varphi_k e^{ikx}$ is an n-component field in a finite cube of volume $V = L^d$ with periodic boundary conditions. The summation $\sum_k$ runs over discrete $\mathbf{k}$ vectors with components $k_j = 2\pi m_j/L, m_j = 0, \pm1, \pm2, \ldots, j = 1, 2, \ldots, d$ in the range $|k_j| \le \Lambda$. Pioneering work on finite-size calculations within this model has been performed previously [3,4] where it was proposed to decompose $\varphi(x)$ as $\varphi(x) = \Phi + \sigma(x)$ and to treat the inhomogeneous modes $\sigma(x) = L^{-d}\sum_{k\neq0}\varphi_k e^{ikx}$ perturbatively while the lowest mode Φ was treated exactly. The order-parameter distribution function $P(\Phi) \equiv P(\Phi, t, L)$ is defined by functional integration over σ as $P(\Phi, t, L) = Z^{-1}\int D\sigma\exp(-H)$, where $Z = \int d^n\Phi\int D\sigma\exp(-H)$. Phenomenological [8] and renormalization-group arguments [9] imply that $P(\Phi)$ has the asymptotic (large L, small $|t|$) scaling form

$$P(\Phi, t, L) = L^{n\beta/\nu} f(\Phi L^{\beta/\nu}, tL^{1/\nu}), \qquad (2)$$

where $t = (T - T_c)/T_c$ is the reduced temperature and β and ν are the bulk critical exponents of the order parameter and the correlation length. While it is straightforward to employ the approach of Ref. [3] to calculate the scaling function f at T_c [5] and above T_c, fundamental difficulties have been shown [7] to arise below T_c for $n > 1$. Unlike the case $n = 1$ below T_c [6], no distribution function $P(\Phi)$ could be determined within the φ^4 model for $n > 1$ because of (spurious) Goldstone singularities [7]. On a qualitative level, one possible solution of this problem may be a low-temperature expansion in $2 + \varepsilon$ dimensions within the nonlinear σ model [3]. On a quantitative level it seems doubtful, however, whether a low-order $d - 2$ expansion can be extrapolated sufficiently well to $d = 3$ to obtain reliable results for finite-size scaling functions in three dimensions. A successful treatment of Goldstone boson related finite-size effects for $n > 1$ has been given previously [10] within a large-volume expansion below T_c. This approach, however, does not include the crossover from the Goldstone dominated behavior for $T < T_c$ to the critical finite-size behavior at $T = T_c$ and for $T \gtrsim T_c$. Here we shall determine $P(\Phi)$ both for $T < T_c$ and $T \ge T_c$ within the φ^4 model directly in three dimensions by a novel approach that includes part of the effect of the $k \neq 0$ modes in a nonperturbative way. Our approach is not restricted to the large-volume regime. The remarkably good agreement of the previous $d = 3$ field theory for $n = 1$ [6] with high-precision MC data for the finite 3D Ising model [11] encourages us to employ the $d = 3$ approach for the φ^4 model also in the present case.

Substituting the decomposition $\varphi = \Phi + \sigma$ into Eq. (1) yields $H = H_0(\Phi) + H'(\Phi, \sigma)$ where

$$H_0(\Phi) = L^d(\tfrac{1}{2}r_0\Phi^2 + u_0\Phi^4), \quad (3)$$

$$H'(\Phi,\sigma) = \int_V d^dx\{\tfrac{1}{2}[r_{0L}\sigma_L^2 + r_{0T}\sigma_{0T}^2 + (\nabla\sigma_L)^2 + (\nabla\sigma_T)^2] + 4u_0\Phi\sigma_L\sigma^2 + u_0\sigma^4\}, \quad (4)$$

with the longitudinal and transverse parameters $r_{0L} = r_0 + 12u_0\Phi^2$, $r_{0T} = r_0 + 4u_0\Phi^2$. Here we have further decomposed $\sigma = \sigma_L + \sigma_T$ into longitudinal and transverse parts that are parallel and perpendicular to the vector Φ, respectively, with $\sigma^2 = \sigma_L^2 + \sigma_T^2$. This yields the distribution function in the form

$$P(\Phi) = (Z^{\text{eff}})^{-1}\exp[-H^{\text{eff}}(\Phi)], \quad (5)$$

$$H^{\text{eff}}(\Phi) = H_0(\Phi) + \Gamma(\Phi) - \Gamma(0), \quad (6)$$

$$\Gamma(\Phi) = -\ln\int D\sigma_L D\sigma_T \exp(-H'), \quad (7)$$

with $Z^{\text{eff}} = \int d^n\Phi\, e^{-H^{\text{eff}}}$. In Eq. (6) the constant $\Gamma(0)$ has been subtracted for convenience. This permits one to let $\Lambda \to \infty$ in the renormalized theory without generating *additive* ultraviolet divergencies of $H^{\text{eff}}(\Phi)$.

The main problem is to develop a perturbation approach to calculate $\Gamma(\Phi)$, Eq. (7). Thus the basic question arises how to split $H'(\Phi,\sigma) = H_1 + H_2$ into an unperturbed part H_1 and a perturbation part H_2. The Gaussian parts of H', Eq. (4), are obviously problematic for $r_0 < 0$ and cannot be used as H_1 because both r_{0L} and r_{0T} become negative for small Φ^2. This problem has been solved perturbatively for $n = 1$ [6] by replacing $\Phi^2 \to M_0^2$ in the longitudinal Gaussian part of H_1 where $M_0^2 = Z_0^{-1}\int d^n\Phi\,\Phi^2 e^{-H_0}$ with $Z_0 = \int d^n\Phi\, e^{-H_0}$. This is not applicable, however, to the transverse part. Although the transverse parameter $\tilde{r}_{0T} = r_0 + 4u_0M_0^2$ remains positive for $r_0 \leq 0$ as long as L is finite, it becomes a dangerous parameter in the bulk limit where $\tilde{r}_{0T}$ vanishes for $r_0 \leq 0$ since M_0^2 approaches the mean-field value $-r_0/4u_0$. This would cause (spurious) Goldstone singularities in a conventional perturbation approach [7].

A simple but important observation is the fact that the distribution function $e^{-H'}$ determining $\Gamma(\Phi)$ is well behaved for large σ not only for $r_0 \geq 0$ but also for $r_0 < 0$ owing to the positivity of the last term $H^{(4)} = \int d^dx\, u_0\sigma^4$ in Eq. (4). Consider $H^{(4)}$ in terms of the Fourier amplitudes $\varphi_k \equiv \sigma_k = \sigma_{Lk} + \sigma_{Tk}$ with $\sigma_0 \equiv 0$,

$$H^{(4)} = u_0L^{-3d}\sum_{kk'k''}(\sigma_k\sigma_{k'})(\sigma_{k''}\sigma_{-k-k'-k''}). \quad (8)$$

The basic idea of our new approach is to include a *tractable* part of this positive term in H_1 such that e^{-H_1} remains well behaved for large σ even for $r_0 < 0$. In constructing H_1 we have been guided by the idea of generalizing the nonperturbative treatment of the $k = 0$ Hamiltonian H_0, Eq. (3), to finite k. We shall show that this is achieved by defining $H_1 = \sum_k[H_k^{(2)} + H_k^{(4)}]$ with

$$H_k^{(2)} = \tfrac{1}{2}L^{-d}[(r_{0L} + k^2)|\sigma_{Lk}|^2 + (r_{0T} + k^2)|\sigma_{Tk}|^2], \quad (9)$$

$$H_k^{(4)} = 3u_0L^{-3d}[|\sigma_{Lk}|^4 + |\sigma_{Tk}|^4], \quad (10)$$

where $H_k^{(4)}$ originates from $H^{(4)}$ for the special cases $k' = -k$, $k'' = k$ or $k' = -k$, $k'' = -k$ or $k' = k$, $k'' = -k$; the factor of 3 in Eq. (10) takes into account the number of possibilities to combine the Fourier amplitudes of Eq. (8) in factors of the form $|\sigma_{Lk}|^4$ and $|\sigma_{Tk}|^4$.

We emphasize that, unlike $H^{(4)}$, the last term of H_1 is a *single* sum that will not contribute to bulk quantities because of the prefactor L^{-3d} of $H_k^{(4)}$. This implies that the coupling of the last term of H_1 is u_0L^{-2d} rather than u_0. It is only the first term of H_1 that yields the usual one-loop bulk contribution to the free energy. Nevertheless, for finite L and $r_0 < 0$, $H_k^{(4)}$ plays the role of a regulator that is crucial in order to ensure the positivity of the small-k part of H_1 in the region $r_{0L} + k^2 < 0$ and $r_{0T} + k^2 < 0$.

In the following we shall neglect H_2. As far as bulk contributions are concerned this corresponds to a one-loop approximation. Then we obtain

$$\Gamma(\Phi) = -\ln\int\prod_{k\neq 0} d\sigma_{Lk}d\sigma_{Tk}\exp(-H_k^{(2)} - H_k^{(4)}). \quad (11)$$

We see that the particular choice of the fourth-order term in H_1 is crucial for the tractability of the non-Gaussian functional integral which is split up into *uncoupled* integrations for each $\mathbf{k} = 2\pi\mathbf{m}/L$. This permits one to treat $H_k^{(4)}$ *nonperturbatively* and leads to the (bare) effective Hamiltonian

$$H^{\text{eff}}(\Phi) = H_0(\Phi) - \frac{1}{2}\sum_{\mathbf{m}\neq 0}\ln\left(\frac{Z_1[y_{0\mathbf{m}}(r_{0L})]}{Z_1[y_{0\mathbf{m}}(r_0)]}\right) - \frac{1}{2}(n-1)\sum_{\mathbf{m}\neq 0}\ln\left(\frac{Z_1[y_{0\mathbf{m}}(r_{0T})]}{Z_1[y_{0\mathbf{m}}(r_0)]}\right), \quad (12)$$

$$y_{0\mathbf{m}}(r) = (2L^{d-4}/3u_0)^{1/2}(rL^2 + 4\pi^2\mathbf{m}^2), \quad (13)$$

$$Z_1[y] = \int_0^\infty ds\, s\exp(-\tfrac{1}{2}ys^2 - s^4). \quad (14)$$

This Hamiltonian is the analytic basis of this Letter. It is applicable for $r_0 \geq 0$ and $r_0 < 0$, for arbitrary L, and is free of Goldstone singularities in the bulk limit as required on general grounds [12] for $O(n)$ invariant quantities.

So far we have not yet dealt with the critical ($r_0 \to r_{0c}$) behavior of $P(\Phi)$. For this purpose we turn to renormalized field theory ($\Lambda \to \infty$) employing dimensional regularization and minimal subtraction at fixed $d<4$ [13]. The renormalized quantities are as usual $\varphi_R = Z_\varphi^{-1/2}\varphi$, $u = \mu^{-\varepsilon}A_d Z_u^{-1} Z_\varphi^2 u_0$, and $r = Z_r^{-1}(r_0 - r_{0c}) = at$ where r_{0c} is the (bulk) critical value of r_0. Using the notation $P(\Phi) \equiv P(r_0 - r_{0c}, u_0, L, \Phi)$ for the bare distribution function Eq. (5) we introduce the renormalized distribution function $P_R(r, u, \mu, L, \Phi_R)$ by

$$P_R = Z_\varphi^{n/2} P(Z_r r, \mu^\varepsilon Z_u Z_\varphi^{-2} A_d^{-1} u, L, Z_\varphi^{1/2}\Phi_R). \quad (15)$$

By integrating the renormalization-group equation for P_R it is then straightforward to derive the finite-size scaling form Eq. (2). Most important is the fact that *the new fourth-order terms $H_k^{(4)}$ in H_1 do not cause new ultraviolet* ($\Lambda \to \infty$) *divergencies beyond one-loop order* as can be shown by studying the large-**k**, i.e., large-**m**, contributions to Eq. (12). Thus it suffices to renormalize $H^{\rm eff}$ by the standard Z factors in one-loop order although $H^{\rm eff}$ contains arbitrary large powers of Φ^2 and u_0/L^{d-4}. The details of the (multiplicative) renormalization of $H^{\rm eff}$ will be given elsewhere [14]. The resulting scaling function defined in Eq. (2) has the structure

$$f(z,x) = \frac{\exp[-F(z,x)]}{\int d^n z \exp[-F(z,x)]}, \quad (16)$$

with $z = \Phi L^{\beta/\nu}$, $x = tL^{1/\nu}$, and

$$F(z,x) = c_2(\hat{x})\hat{z}^2 + c_4(\hat{x})\hat{z}^4 - \frac{1}{2}\sum_{\mathbf{m}\neq 0} \ln\frac{Z_1\{y_\mathbf{m}[\tilde{r}_L(\hat{z},\hat{x})]\}}{Z_1\{y_\mathbf{m}(\tilde{r}_L(0,\hat{x}))\}} - \frac{1}{2}(n-1)\sum_{\mathbf{m}\neq 0}\ln\frac{Z_1\{y_\mathbf{m}[\tilde{r}_T(\hat{z},\hat{x})]\}}{Z_1\{y_\mathbf{m}[\tilde{r}_T(0,\hat{x})]\}}. \quad (17)$$

Here $\hat{x} = Q^* t(L/\xi_0)^{1/\nu}$ and $\hat{z} = (2Q^*)^\beta(\Phi/A_M) \times (L/\xi_0)^{\beta/\nu}$ are convenient dimensionless scaling variables normalized to the asymptotic amplitudes A_M and ξ_0 of the bulk order parameter $M_{\rm bulk} = A_M|t|^\beta$ below T_c and of the bulk correlation length $\xi = \xi_0 t^{-\nu}$ above T_c. The well-known bulk parameter $Q^*(n)$ [13] will be given below. In three dimensions we obtain

$$y_\mathbf{m}(\tilde{r}(\hat{z},\hat{x})) = [6\pi u^*\tilde{\ell}(\hat{x})]^{-1/2}[\tilde{r}(\hat{z},\hat{x})\tilde{\ell}(\hat{x})^2 + 4\pi^2\mathbf{m}^2], \quad (18)$$

$$\tilde{r}_L(\hat{z},\hat{x}) = \hat{x}\tilde{\ell}(\hat{x})^{-1/\nu} + (3/2)\tilde{\ell}(\hat{x})^{-2\beta\nu}\hat{z}^2, \quad (19)$$

$$\tilde{r}_T(\hat{z},\hat{x}) = \hat{x}\tilde{\ell}(\hat{x})^{-1/\nu} + (1/2)\tilde{\ell}(\hat{x})^{-2\beta\nu}\hat{z}^2, \quad (20)$$

which are the dimensionless renormalized counterparts of $y_{0\mathbf{m}}$, $r_{0L} - r_{0c}$, and $r_{0T} - r_{0c}$, respectively. The coefficients $c_2(\hat{x})$ and $c_4(\hat{x})$ read for $d = 3$

$$c_2(\hat{x}) = (64\pi u^*)^{-1}\hat{x}\tilde{\ell}(\hat{x})^{3-(2\beta+1)/\nu}[1 + 4(n+2)u^*], \quad (21)$$

$$c_4(\hat{x}) = (256\pi u^*)^{-1}\tilde{\ell}(\hat{x})^{3-4\beta/\nu}[1 + 4(n+8)u^*], \quad (22)$$

where $u^*(n)$ is the known [13] fixed point value of the renormalized coupling u. The auxiliary scaling function $\tilde{\ell}(\hat{x})$ of the flow parameter is determined by

$$\tilde{\ell}(\hat{x})^{3/2} = (4\pi u^*)^{1/2}\{\tilde{y}(\hat{x}) + 12\vartheta_2[\tilde{y}(\hat{x})]\}, \quad (23)$$

$$\tilde{y}(\hat{x}) = (4\pi u^*)^{-1/2}\tilde{\ell}(\hat{x})^{3/2-1/\nu}\hat{x}, \quad (24)$$

$$\vartheta_2(y) = \frac{\int_0^\infty ds\, s^{n+1}\exp(-\frac{1}{2}ys^2 - s^4)}{\int_0^\infty ds\, s^{n-1}\exp(-\frac{1}{2}ys^2 - s^4)}. \quad (25)$$

The sums $\sum_{\mathbf{m}\neq 0}$ in Eq. (17) can be evaluated by using the prescriptions of dimensional regularization [15] and by computing their finite contributions in three dimensions numerically [14]. Our result for the universal function $f(z,x)$ requires no adjustment of parameters (other than the *bulk* amplitudes A_M and ξ_0). Since $f(z,x)$ depends only on $|z|$ (rather than on the vector z) and because of $d^n z = g(n)d(|z|^n)$ with $g(n) = 2\pi^{n/2}[n\Gamma(n/2)]^{-1}$, we have plotted $f_g(z,x) = g(n)f(z,x)$ vs $|z|^n$ in Fig. 1 for $n = 2$ and 3. The corresponding values of $Q^*(n)$ and $u^*(n)$ are [13] $Q^* = 0.939, 0.937$ and $u^* = 0.0362, 0.0328$; for the bulk critical exponents we take $\beta = 0.344, 0.365$ and $\nu = 0.671, 0.705$, respectively [16–19].

In order to test these predictions of our theory we have performed MC simulations for $O(n)$ symmetric spin models which are believed to belong to the same universality class as the $O(n)$ symmetric φ^4 model. There have been successful comparisons of MC simulations for the 3D *XY* [20] and Heisenberg models [21] with the results of Ref. [10]. They did not include, however, the distribution function $P(\Phi)$. Specifically, $P(\Phi)$ of the φ^4 model corresponds to the distribution function $P(\mathbf{M})$ of the magnetization $\mathbf{M} = N^{-3}\sum_i \mathbf{s}_i$ of the *XY* ($n = 2$) and Heisenberg ($n = 3$) models on a cubic N^3 lattice. Their (nearest-neighbor) Hamiltonian reads $H = -K\sum \mathbf{s}_i \cdot \mathbf{s}_j, 1K > 0$, where $\mathbf{s}_i$ is an n-component unit vector on the lattice site i. Like $f(z,x)$, $P(\mathbf{M})$ depends only on $M = |\mathbf{M}|$, and the probability dW to find $\mathbf{M}$ in the element $d^n\mathbf{M}$ can be written as $dW = P(\mathbf{M})d^n\mathbf{M} = \tilde{P}(M)d(M^n)$ with $\tilde{P} = g(n)P$. We have obtained the distribution

$$\tilde{P} = \frac{1}{Z}\int D\mathbf{s}\, e^{-H}\delta(|N^{-3}\sum_i \mathbf{s}_i|^n - M^n), \quad (26)$$

with $Z = \int D\mathbf{s}\, e^{-H}$ by generating spin configurations according to the distribution e^{-H} using Wolff's cluster algorithm [22] and making histograms with the values for M^n. With L,A_M, and ξ_0 taken in units of the lattice constant, $\tilde{P}$ is related to the scaling function in Eq. (16) as $\tilde{P}(M,t,L) = L^{n\beta/\nu}g(n)f(z,x)$.

Figure 1 shows that the MC data for various lattice sizes are in good agreement with the theoretical predictions both at T_c and below T_c. (Similar agreement is found above T_c.) The different steepness of f at T_c near $z = 0$ for $n = 2$ and $n = 3$ is well described by the theory. The qualitative difference between the increasing ($n = 2$) and decreasing ($n = 3$) maximum below T_c is an unexpected n dependence of the order-parameter distribution function.

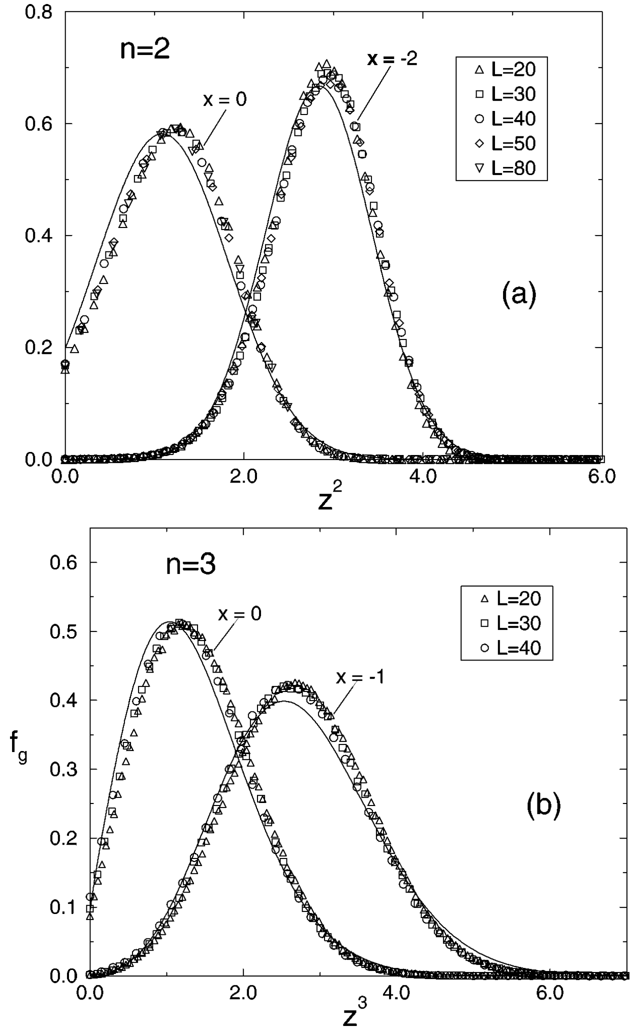

FIG. 1. Theoretical predictions (solid lines) and MC data for the scaling function $f_g = g(n)f(z,x)$ at T_c ($x = 0$) and below T_c ($x < 0$): (a) for the XY model [$\xi_0 = 0.498$ [17], $A_M = 1.217$, $g(2) = \pi$] and (b) for the Heisenberg model [$\xi_0 = 0.484$ [18], $A_M = 1.118$, $g(3) = 4\pi/3$], with $z = \Phi L^{\beta/\nu}$ and $x = tL^{1/\nu}$, in units of the lattice constant. The normalization is $\int_0^\infty f_g d(|z|^n) = 1$.

Having established the shape of $f(z,x)$ we are in the position to determine the finite-size effects on various important thermodynamic quantities such as susceptibility, specific heat, and magnetization. A generalization to finite external ordering field [14], different geometries, and boundary conditions will be studied in the future. Our idea of a nonperturbative treatment of the $k \neq 0$ modes may also open up the possibility of entering the unexplored area of finite-size *dynamics* of $O(n)$ symmetric systems.

Our results can, of course, be applied also to the simpler case $n = 1$. Good agreement with recent MC data for $P(\Phi)$ of the 3D Ising model above and below T_c [2] is found [14]. It turns out that the leading term of an expansion of our present theory around $\Phi^2 = M_0^2$ coincides with the previous version of the $n = 1$ theory [6,11].

Support by Sonderforschungsbereich 341 der Deutschen Forschungsgemeinschaft is acknowledged.

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